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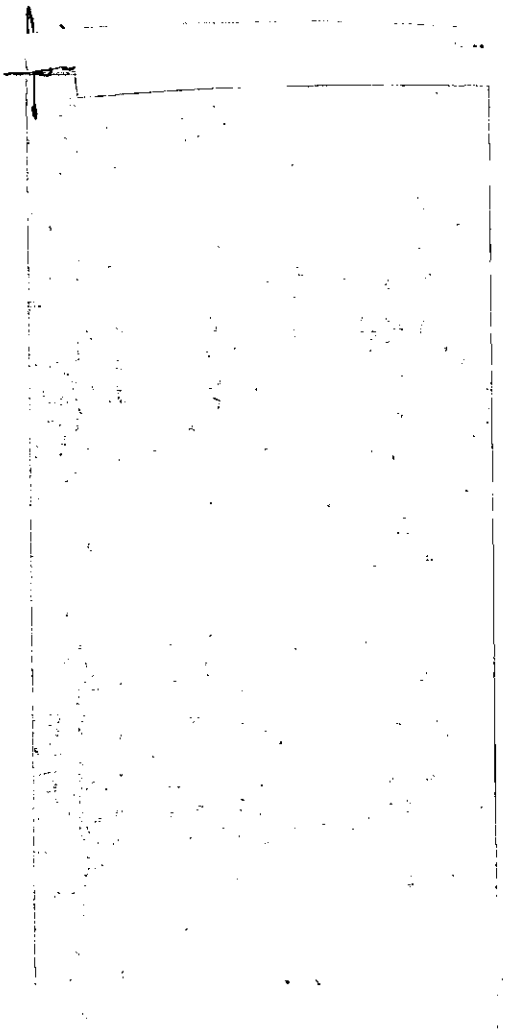

A QUANTUM MECHANICAL CELL MODEL OF A DENSE BOSON SYSTEM

A THESIS

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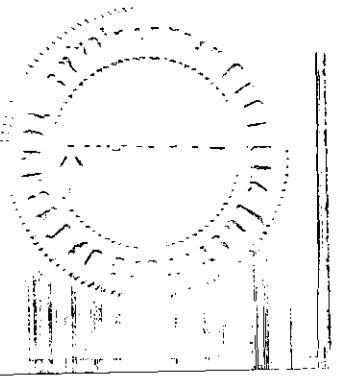

A QUANTUM MECHANICAL CELL MODEL OF A DENSE BOSON SYSTEM

Approved:

H. A. Gersch, Chairman

C. H. Braden

R. H. Kasriel

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SUMMARY

Unlike solids and gases, liquids do not allow a general calculation of their thermodynamic properties. The study of certain solids is a relatively tractable problem due in large part to the small oscillations of the individual molecules, while a dilute gas at rather high temperature, for example, is a fairly elementary system since, on the average, constituent molecules are so far apart that they exert negligible forces on each other. Due to the presence of strong interactions between the molecules of a liquid and simultaneously large vibrations compared with those existing in the case of a harmonic solid, more details of the intermolecular forces are required than is needed to calculate thermodynamic quantities for either a solid or a gas. However, a study of the properties of the liquid state can be made in general form near absolute zero. Although in practice only the isotopes of helium can remain liquid down to absolute zero, the principles involved in low-temperature studies are of considerable interest and have attracted the attention of numerous investigators in recent times. At extremely low temperatures, quantum effects are important and helium is, therefore, a "quantum liquid."

In calculating thermodynamic properties it is necessary to know the energy spectrum of the given physical system. Owing to the particularly weak interaction between the atoms of helium, early investigations treated helium four as an ideal Bose-Einstein gas, at least to a first approximation; the qualitative similarity between the λ-transition and

the Einstein condensation added stature to this approach. Subsequent refinements were introduced to treat a dilute nonideal Bose gas; these lead to the energy spectrum for weakly excited states at small momenta, and it was found that the excitations correspond to normal sound waves--that is, are phonons. The energy spectrum associated with phonon excitations possesses the property of superfluidity, which is a characteristic of liquid helium at temperatures below about 2.2°K. Since conventional perturbation methods when applied to this problem introduced formal complications, new perturbation theories using the second quantization formalism were expounded. The same problem has also been considered dealing directly with a pair-type wave function in configuration space and employing the theory of cluster expansions which originated in statistical mechanics. Recently, the properties of a Boson system have been studied by means of the familiar Green's functions of quantum field theory.

Procedures heretofore presented in the literature and applicable to many-particle Boson systems cannot in general be used at high densities and therefore inherently possess a fundamental inadequacy in regard to quantum liquids such as helium four. Since, for classical liquids, lattice or cell-model theories have provided semiquantitative agreement with experimentally determined thermodynamic properties, it is the purpose of the present investigation to develop a quantum mechanical analogue for a system of closely-packed, interacting Bose particles, and to employ the model to derive certain of its low-temperature properties. Since the average molecule in the liquid state is presumably closely confined by its nearest neighbors, a solid-like state is used as a point of departure.

Accordingly, cells of size equivalent to the volume per particle are chosen to ensure that there will be on the average of one particle per cell. The zero-point energy of each atom of helium at low temperatures indicates that the volume of a cell is much greater than the "hard sphere" volume of the molecule; therefore, multiple occupation of a cell is to be expected. The limitation is made to no more than double occupancy, a restriction which is not severely prohibitive in the classical case. All effects which are small in the limit of infinite particle number and infinite enclosing volume are neglected. Quantized field theory, or the formalism of second quantization, is employed throughout.

Expansion of the field operator appearing in the Hamiltonian in an orthogonal set of plane wave states is customary at low density. Here, instead, the expansion is performed in a set of Kronecker δ functions located at respective cell centers. This simplified set of states has the advantage of facilitating the mathematical development, but fails to provide fine-structure details. Nevertheless, properties of the system near ground state should not be appreciably affected. The Hamiltonian of the system is next expressed in terms of creation and destruction operators for particles localized in cells, a description which is almost the inverse of the plane-wave formalism. Off-diagonal terms now appear in the kinetic energy expression and correspond to particle wanderings from cell to cell, resulting in decreased localization and a consequent reduction in the kinetic energy of localization. A density-dependent, effective interaction between particles is defined which, for highly repulsive forces at small volumes, virtually locks the particles in their respective cells. It is shown that the well-known results for noninteracting

particles and for low-density Boson systems with finite interaction potentials can be easily obtained from the derived cell-model Hamiltonian.

Subsequent to the formulation of a quantum mechanical lattice model suitable for a description of compact Bose ensembles, Rayleigh-Schrödinger perturbation theory is employed to calculate the ground state energy of a one-dimensional particle array. An exact energy expansion is performed through sixth order in which both linked and unlinked contributions are taken into account. The expansion parameter represents the ratio of kinetic energy of localization to potential energy for double occupancy and is a measure of the system confinement, the smaller this parameter the less the tendency of particle wanderings. A pictorial representation of the matrix elements involved in the perturbation treatment is introduced to aid in the calculations and discussions; these pictures correspond closely to the well-known Brueckner diagrams. A separate study is also made of the energy contribution, to infinite order of perturbation, from linked single pair interactions, the major contributors to the ground state energy. This analysis is accomplished by identifying the problem with that for a restricted random walk on a one-dimensional lattice, the solution of which is known. A propagator modification applicable in the case of nearest-neighbor hole-double combinations is next introduced and utilized to determine the corresponding contribution to the ground state energy. An identical result is subsequently derived by solving the Schrödinger equation using a nearest-neighbor hole-double state vector. By means of the foregoing analysis, the effective energy of a hole-double pair at nearest-neighbor distance is ascertained, as well as the expected number of such pairs.

For linked single pair excitations in a two-dimensional Boson system of closely-packed particles, the problem is again approached from the standpoint of a restricted random walk on a periodic square lattice. Since a solution of the latter problem is not to be found in the available literature, an approximate energy expansion is derived by solving a simplified version of the generalized two-dimensional walk problem apropos of the Boson system. Other specialized cases are also treated such that both an upper and a lower bound on the ground state energy for a two-dimensional system can be had. Although the primary purpose in mind governing the choice of these special cases was the solvability of ensuing mathematical problems, the somewhat arbitrary energy bounds thus calculated are found, surprisingly, to provide a relatively narrow bandwidth for the energy spectrum.

To discuss results and indicate trends, a plot versus the expansion or confinement parameter is presented of the ground state energy for both the one- and the two-dimensional models. Since even elemental unrestricted random walk problems as applied to three-dimensional lattice networks have not been solved in closed form, no analytical attempt is made to study directly a Boson system in more than two dimensions. To best illustrate and discuss conclusions derivable from the theoretical development a simple effective interaction potential is assumed and the ground state energy is plotted as a function of reciprocal density. As anticipated, a lowering of the energy spectrum is realized with increased dimensionality of the system, and the ground state energy is, in all cases, a monotonic increasing function of density. Of course, a fundamental mathematical approach to the three-dimensional Boson lattice is

much to be desired. To this end, a fruitful investigation involves determination of a unitary transformation which diagonalizes the derived cell-model Hamiltonian. Further studies based on the foundations laid here involve a refined description of the singlet probability density, determination of the indigeneous ground state wave function for the cell-model Boson system and, as well, an excited-state function, and calculation of the relative effects attributable to linked multiple pair interactions.

CHAPTER I

INTRODUCTION

The microscopic physical processes which contribute to the properties and behavior of the liquid state of matter seem to be little understood at present. Helium II near absolute zero appears to be the only liquid whose behavior it has thus far been possible to quantitatively understand, at least in part. It consists of an ensemble of He^4 atoms which obey Bose-Einstein statistics (and are therefore designated as Bosons), and is truly a quantum liquid. Since the forces between helium atoms are of a very weak nature, early investigations treated liquid helium as being an ideal Bose-Einstein system, at least to a first approximation. This point of view was enhanced by the superficial similarity between the λ-transition and the Einstein condensation (1)(2). However, any reasonable theory of the liquid state must, of course, consider the interaction forces. Landau (3) and Feynman (4) explained the thermodynamic behavior of liquid helium four on the basis of a phenomenological model. To develop a theory based on first principles, later studies have had as their purpose investigation of interacting Boson systems with a variety of characteristics.

In approximating the helium four atom by the classical hard sphere, Huang, Yang, Luttinger, and Lee (5)(6)(7) considered the problem of a dilute collection of particles interacting via a two-body hard-sphere potential, where the latter is first formulated in terms of a

pseudopotential which, in turn, is treated as a perturbation. Brueckner and Sawada (8) have presented a general theory applicable to Boson systems at low temperature and appropriate to the study of strong interactions. A procedure was developed by them to deal with the region in which the usual perturbation theory fails. The results were applied to a hard-sphere system at both low and "high" density (8)(9). Some difficulties arise in the foregoing treatments for the case of potentials which are repulsive at small distances but have longer-ranged regions of attraction. However, Abe (10) has applied a modified Brueckner theory to such cases as an attractive square-well potential with hard-core repulsion, the Sutherland and the Lennard-Jones potentials, and has obtained the corresponding ground state energy of a Bose particle system at low densities. In addition, Abe (11) has generalized somewhat the pseudopotential method to include certain arbitrary potentials and has derived therefrom the ground state energy of a Bose system with Lennard-Jones potential. Huang (12) has also given an example in which an extension of the pseudopotential approach is made to the problem of weak attraction in addition to hard-core repulsion. Other treatments involving, for the potential, hard-core repulsion together with a weak attraction include those of Eleonskii and Zyrianov (13). Recently the pseudopotential and Brueckner methods have been used to calculate further terms in the low-density expansion of the ground state energy (14)(15) and in the low-lying excitation energies of a Bose gas of hard spheres (16). It is noted that Lee and Yang (17)(18) have also developed the "method of binary collision expansion" which expands the grand partition function

of an N-body system, whose particles interact through a general two-body potential, in terms of a quantity which remains finite for singular potentials and which bears a similarity to the "t matrix" in the theories of Brueckner and Levinson (19)(20). A noteworthy summary of present work on Bose hard-sphere systems, as well as on many-body problems in general, was made at the recent International Congress on Many-Particle Problems (21).

Bogoliubov and Zubarev (22)(23)(24) have used a method of auxiliary variables to obtain the ground state wave function of a Bose system with weak interactions and have determined the energy spectrum for the system. By taking into account certain terms of the Hamiltonian neglected by the previous authors, Sanochin (25) has extended their results for the energy of the ground state and that of single Boson excitations, and has made possible the inclusion of singular potentials. The behavior of a nonideal Bose system close to the phase transition has been studied by Zubarev and Tserkovnikov (26) by employing a model Hamiltonian which is of the same type as that given by Brueckner and Sawada (8) and which is a special case of that appearing in Bogoliubov's theory of superfluidity (22). An increase in the density of interacting particles in a Bose gas results in a decrease in the number of particles in the condensate, and Geilikman (27) has concentrated on the case for which this number is finite but small.

Many-particle systems have of late been scrutinized with the aid of the familiar Green's functions of quantum field theory (28)(29)(30)(31)(32). The one-particle Green's function determines the average value of all one-body operators, while two-particle Green's functions give averages

of two-body operators. Application of Green's functions is particularly useful in those cases where one can sum some class of perturbation-theory diagrams, but the method is not directly based upon perturbative theories and thus avoids some of the peculiar difficulties attendant upon the latter. Green's function techniques have been applied to a system of interacting Bosons by Beliaev (33)(34) and by Hugenholtz and Pines (35). It is noted that the Bose many-particle system has also been treated by dealing directly with the wave function in configuration space, using the theory of cluster expansions (36)(37). Variation with respect to a parameter in a trial function of the pair-excitation type for the ground state has been shown to yield a ground state energy close to that obtained from perturbation theory (38)(39)(40). Complete equivalence of the cluster integral method and the pair approximation in perturbation theory has recently been demonstrated (41).

The foregoing survey of a particular class of quantum mechanical many-body problem, namely that of a system of interacting Bosons, is by no means exhaustive, but serves to indicate some approaches to the problem, the purpose of which is the eventual understanding of liquid helium four as well as the development of new mathematical methods with which to treat interacting systems in general. As one perhaps can surmise, the procedures presented in the literature are not applicable, for the most part, in the high-density region and therefore tend to be fundamentally inadequate in describing the properties of certain quantum liquids such as helium four. For classical liquids, qualitative or semiquantitative agreement with experimental thermodynamic properties has been achieved using lattice theories of the liquid state (42)(43). In these theories,

the liquid state is represented by a model of the solid state--that is, the crystalline state rather than the gaseous state is used as the point of departure. It is argued that the average molecule in a liquid is presumably confined in a "cell" or "cage" formed by its nearest neighbors, and is only very rarely involved in excursions outside of the cell.

Lennard-Jones and Devonshire (44), as well as Hirschfelder, et al. (45), have developed a cell method for the liquid state which makes possible an approximate evaluation of the partition function in terms of the intermolecular forces between molecules. Owing to the confinement of every molecule in its motion to one particular cell, from which all others are excluded, the foregoing model takes insufficient account of the correlation between the motions of molecules in neighboring cells. The method has been improved and generalized by many investigators, and a critical survey of these refined approaches has been presented by de Boer (46). An interesting attempt to account for the disorder in the liquid state has been made by Janssens and Prigogine (47) and by Pople (48) through the introduction of multiple occupied cells. Here states are considered in which there are two molecules in the same cell. These fluctuations in the occupation number, which might be interpreted as microscopic density fluctuations, play an especially significant role at small densities. In particular, Prigogine and Philippot (49) have attempted to account for many of the properties of liquid helium on the basis of these microscopic occupation fluctuations. The cell method of Lennard-Jones has also been generalized in a different way (50) by considering systematically the motion of two or more neighboring molecules in a "cell-cluster" of two or more neighboring cells, considered as one large cell

shared collectively by the molecules in the cell-cluster. Quantum mechanical exchanges of neighboring molecules are treated on the basis of this model. Although no calculations with a realistic intermolecular field have been made with this theory, a number of examples using simplified interaction potentials (51)(52)(53)(54) revealed that taking into account the correlations between motions of molecules in two nearest-neighbor cells alone leads to a considerable increase in entropy over that realized from single cell theory. A generalization of the cell-cluster theory for a pure liquid to the case of a binary solution has lately been published (55).

It is the purpose of the present work to study the low-temperature properties of a dense system of Bose particles with finite interaction potentials. Since the cell-model description appears to provide reasonable utility where classical liquids are concerned, a quantum mechanical counterpart is developed here and applied to a close-packed Boson system. Cells of size equivalent to the specific volume are chosen to ensure that, on the average, there will be one particle in each cell. The number of the particles and the volume in which they are enclosed is assumed to be so large that all effects which are small in the limit of infinite number and volume can be neglected. Particle density, however, remains finite. Since, classically, allowing for double occupation of cells corrects the major deficiency of "single-occupation" cell theories, the occupation of a cell is herein restricted to a maximum of two particles. At liquid densities, the singlet probability density inside a singly-occupied cell will presumably have a rather high maximum at the center of the cell and fall off very rapidly near the edges of the cell. Instead of considering

in detail the fine structure of the model with its concomitant mathematical burdens, one here assigns a constant amplitude to the singlet probability throughout a cell. Ground state and near ground state properties should not be appreciably affected by this simplification.

In Chapter II, the formulation of the quantum mechanical cell model is presented using the concise formalism of second quantization, and an appropriate Hamiltonian operator for a dense Boson system is derived. Following a brief qualitative discussion of the nature of the Hamiltonian, the latter is used to deduce several well-known results as a test of its general validity.

In Chapter III, the ground state energy of a dense one-dimensional Boson system based on the cell model is studied with the aid of Rayleigh-Schrödinger perturbation theory. Linked and unlinked contributions through sixth order are separately calculated, as well as the contributions to infinite order of linked single pair propagations. Modification of the propagator to include all nearest-neighbor hole-double pairs is also discussed.

Chapter IV deals with the ground state wave function descriptive of nearest-neighbor hole-double combinations. A solution of the Schrödinger equation for the determination of the energy eigenvalues in this special case is presented.

Calculation of an approximate ground state energy for a dense two-dimensional Boson system is contained in Chapter V, together with a determination of upper and lower energy bounds. The results of the aforementioned analyses, as well as those for the one-dimensional particle array, are summarized and discussed in Chapter VI. Recommendations for further studies are included in this chapter.

CHAPTER II

FORMULATION OF THE QUANTUM CELL MODEL

A system of spinless, non-relativistic Boson particles is considered to be enclosed in a large box. Both the number N of interacting particles and the volume Ω of the box are assumed to be so large that all effects which are small in the limit $N \to \infty$ and $\Omega \to \infty$ can be neglected. The limit is taken in such a way that the particle density $\rho = \frac{N}{\Omega}$ remains finite. In the formalism of second quantization, the Hamiltonian operator for such a system is represented by

$$H = \frac{\hbar^2}{2m}\int \nabla\psi^*(r)\cdot\nabla\psi(r)d\tau + \frac{1}{2}\int \psi^*(r)\psi^*(r')\, U(r-r')\, \psi(r)\psi(r')d\tau\, d\tau' \tag{1}$$

where $\psi^*(r)$ and $\psi(r)$ are, respectively, creation and destruction operators for a particle positioned at r, and $U(r-r')$ is the interaction operator for particles at r and r'. The corresponding number operator representing the total number of particles is

$$N = \int \psi^*(r)\psi(r)d\tau \tag{2}$$

and the commutation relations for Bosons are

$$[\psi(r),\ \psi(r')] = [\psi^*(r),\ \psi^*(r')] = 0 \tag{3a}$$

$$[\psi(r),\ \psi^*(r')] = \delta(r-r'). \tag{3b}$$

For systems of low density, the field operator $\psi(r)$ is customarily expanded in a complete set of plane wave states. Since the system of interest here is one of close packing, an expansion in some set other than the plane wave is obviously highly beneficial. Accordingly, the box of Boson particles is divided into cells of size τ equal to the specific volume $\frac{1}{\rho}$. As evidenced further on, this choice of cell size has the distinct advantage of yielding an effective interaction which depends on density. The adoption of a model in which the particles are localized in cells suggests an expansion of the field operator in a complete orthogonal set of functions $f(r-r_j)$ centered about the cell j:

$$\psi(r) = \rho^{\frac{1}{2}} \sum_{r_j} b_{r_j} f(r-r_j) . \tag{4}$$

For long wave lengths--that is, wave lengths which are long compared to a cell size, the Kronecker δ function defined by

$$\delta_{r,r_j} = \begin{cases} 1, \text{ if } r \text{ is in cell centered on } r_j \\ 0, \text{ otherwise} \end{cases} \tag{5}$$

is chosen as a convenient orthogonal set. Although the field operator is hereby assigned a constant amplitude throughout a cell (resulting in the loss of some detail regarding the fine structure of the model), the low-lying energy levels should still be obtainable with precision.

The field operator $\psi(r)$ now has the form

$$\psi(r) = \rho^{\frac{1}{2}} \sum_{r_j} b_{r_j} \delta_{r,r_j} \tag{6}$$

as opposed to the usual Fourier decomposition. Equation (6) is used to find the commutation relations for the cell occupation operators b_{r_j}. Introduction of (6) into (3b) yields

$$\rho \sum_{r_j} \sum_{r_k} \delta_{r,r_j}\, \delta_{r',r_k}\, (b_{r_j}\, b^*_{r_k} - b^*_{r_k}\, b_{r_j}) = \delta(r - r') \,.$$

Multiplication of the above on both sides by δ_{r',r_ℓ} and integration over r' gives

$$\sum_{r_j} \delta_{r,r_j}\, (b_{r_j}\, b^*_{r_\ell} - b^*_{r_\ell}\, b_{r_j}) = \delta_{r,r_\ell} \,.$$

A multiplication of this result by δ_{r,r_m} and subsequent integration over r leads to the commutator

$$[b_{r_m},\, b^*_{r_\ell}] = \delta_{r_m,r_\ell} \,. \tag{7}$$

In similar fashion, b_{r_m} and b_{r_ℓ} are found to commute, as well as $b^*_{r_m}$ and $b^*_{r_\ell}$. By comparison with quantum field theory (56) it is evident that $b^*_{r_j}$ and b_{r_j} are creation and annihilation operators, respectively, for particles in the j-th cell. The number operator of Equation (2) becomes in terms of these new operators

$$N = \sum_{r_j} b^*_{r_j}\, b_{r_j} = \sum_{r_j} n_{r_j} \tag{8}$$

where $n_{r_j} = b^*_{r_j} b_{r_j}$ is the occupation number of the cell at r_j.

Equation (6) is now introduced into the Hamiltonian of Equation (1) to express the latter in the new operator notation. A finite difference approximation (see, for example, Hildebrand (57)) is adopted for the operator $\nabla^2 b_{r_j} \delta_{r,r_j}$

$$\nabla^2 b_{r_j} \delta_{r,r_j} = \frac{1}{r_o^2} \left[b_{r_j} \delta_{r,r_j+r_o} - 2b_{r_j} \delta_{r,r_j} + b_{r_j} \delta_{r,r_j-r_o} \right]$$

where r_o^3 is the volume τ of a cell, which is the reciprocal of the particle density ρ. It is noted that the difference representation written above inherently implies a one-dimensional particle model. This simplification here facilitates the subsequent perturbation treatment; a two-dimensional periodic lattice structure is later considered as a natural extension of the results predicated upon the linear array. The kinetic energy operator T of Equation (1) is

$$T = -\frac{\hbar^2}{2m} \int \psi^*(r) \nabla^2 \psi(r) d\tau$$

which becomes in view of the finite difference approximation noted above

$$T = -\frac{\hbar^2}{2m} \int d\tau \left\{ \sum_{r_k} \rho^{\frac{1}{2}} b^*_{r_k} \delta_{r,r_k} \right\} \rho^{\frac{2}{3}} \left\{ \sum_{r_j} \rho^{\frac{1}{2}} (b_{r_j} \delta_{r,r_j+r_o} - 2b_{r_j} \delta_{r,r_j} + b_{r_j} \delta_{r_j-r_o}) \right\} = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} \sum_{r_j} b^*_{r_j} b_{r_j} - \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \sum_{r_j} (b^*_{r_j} b_{r_j+r_o} + b^*_{r_j} b_{r_j-r_o}) . \quad (9)$$

Reference to Equation (8) reveals that the first term appearing on the right in Equation (9) above is simply the sum of n_{r_j} times the minimum kinetic energy for a particle in a square well potential of spatial extent r_o (58). The second term on the right side of (9)--the off-diagonal element--represents the drifting of particles into neighboring cells, where $b^*_{r_j} b_{r_j+r_o}$ and $b^*_{r_j} b_{r_j-r_o}$ are so-called "shift" operators. This latter term effects a decrease in the kinetic energy from its value for localized particles, a result which one would anticipate because the shifting of particles spreads out the wave function which in turn implies a reduced kinetic energy.

A second step in the reduction of Equation (1) to its equivalent representation involving the aforementioned shift operators is the description of the potential energy operator V in terms of creation and destruction operators, where V is the second term on the right in Equation (1). Substitution of (6) into this term and subsequent evaluation of a double summation leads to

$$V = \frac{\rho^2}{2} \sum_{r_j} \sum_{r_k} \sum_{r_\ell} \sum_{r_m} b^*_{r_j} b^*_{r_k} b_{r_\ell} b_{r_m} \times$$

$$\int U(r-r') \delta_{r,r_j} \delta_{r',r_k} \delta_{r,r_\ell} \delta_{r',r_m} \, d\tau \, d\tau'$$

$$= \frac{1}{2} \rho^2 \sum_{r_j} \sum_{r_k} b^*_{r_j} b^*_{r_k} b_{r_j} b_{r_k} \int_{\substack{r \text{ in cell } j \\ r' \text{ in cell } k}} U(r-r') d\tau \, d\tau' . \qquad (10)$$

Equation (10) is rewritten

$$V = \frac{1}{2}\rho^2 \sum_{r_j} b^*_{r_j} b^*_{r_j} b_{r_j} b_{r_j} U_o + \frac{1}{2}\rho^2 \sum_{r_j \neq r_k} b^*_{r_j} b_{r_j} b^*_{r_k} b_{r_k} U_{jk} \tag{11}$$

where the effective interaction potentials U_o and U_{jk} are defined as†

$$\begin{aligned} U_o &= \int U(r-r')\,d\tau\, d\tau', \; r \text{ and } r' \text{ in one cell} \\ U_{jk} &= \int U(r-r')\,d\tau\, d\tau', \; r \text{ and } r' \text{ in different cells } (j \neq k) \,. \end{aligned} \tag{12}$$

The first term on the right in (11) is simplified through the use of the commutation relation in Equation (7). Thus

$$b^*_{r_j} b_{r_j} = b_{r_j} b^*_{r_j} - 1$$

$$b^*_{r_j} b^*_{r_j} b_{r_j} b_{r_j} = b^*_{r_j} (b_{r_j} b^*_{r_j} - 1) b_{r_j}$$

$$= b^*_{r_j} b_{r_j} (b^*_{r_j} b_{r_j} - 1)$$

$$= n_{r_j}(n_{r_j} - 1) \,.$$

Now Equation (11) reads

---

†Equations (12) impose a limitation to integrable potentials. The inclusion in the function $f(r-r_j)$ appearing in Equation (4) of a local function for each cell would obviate this restriction. Mathematical expediency guided the approach taken herein.

$$V = \frac{\rho^2 U_o}{2} \sum_{r_j} n_{r_j} (n_{r_j} - 1) + \frac{\rho^2}{2} \sum_{r_j \neq r_k} n_{r_j} n_{r_k} U_{jk} \, . \qquad (13)$$

As mentioned previously, the particular choice of cell size leads to an effective interaction which depends on the particle density, a result evidenced in Equations (12). By proper adjustment of parameters, any interaction from strongly repulsive to strongly attractive can be considered. In particular, a rather accurate representation of a known interaction potential is feasible.

In all ensuing work, the term involving U_{jk} in Equation (13) will be neglected on the following basis. Since physically realizable potentials are of relatively short range, the integration over cells in the second of Equations (12) will yield a relatively insignificant contribution as compared to that given by the first of Equations (12). Combining then the principal part of (13) with (9) gives the Hamiltonian operator as follows:

$$H = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} \sum_{r_j} b^*_{r_j} b_{r_j} - \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \sum_{r_j} (b^*_{r_j} b_{r_j + r_o} + b^*_{r_j} b_{r_j - r_o})$$

$$+ \frac{\rho^2 U_o}{2} \sum_{r_j} n_{r_j} (n_{r_j} - 1) \, . \qquad (14)$$

An inverse symmetry exists in Equation (14) from that encountered when the field operator is expanded in conventional plane waves. Here the

potential energy operator is diagonal in occupation number representation while the kinetic energy operator is not.

A brief qualitative discussion of the Hamiltonian applicable to the cell model adopted here will now be presented. For highly repulsive interactions corresponding to a high density ρ, U_o will be relatively large, or

$$\frac{\rho^2 U_o}{2} \gg \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} .$$

Thus particles will be inhibited from shifting about and, as expected, a "locked in" behavior ensues. The ground state of the system then corresponds to one particle per cell with little or no wanderings. In the opposite extreme of low densities

$$\frac{\rho^2 U_o}{2} \ll \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m}$$

and the kinetic energy portion of the Hamiltonian predominates. Now severe particle wanderings occur. If U_o is allowed to become negative, the potential energy again dominates but in such a manner as to allow large fluctuations in particle numbers per cell. Unless the fluctuations are limited in this extreme, the whole system collapses.

It is of interest to conclude the cell model development by deriving several known results using the Hamiltonian operator given in Equation (14). First, $\langle V \rangle$ for the ground state at low density is computed:

$$\langle V \rangle = \frac{\rho^2 U_o}{2} \sum_{r_j} \langle n_{r_j} (n_{r_j} - 1) \rangle$$

$$= \frac{N\rho^2 U_o}{2} (\langle n_{r_1}^2 \rangle - \langle n_{r_1} \rangle) .$$

To compute $\langle n_{r_1}^2 \rangle$, one takes the average number of particles $\langle n_{r_1} \rangle$ in any single cell to be unity and expresses the actual number per cell by the Poisson distribution function. Hence, the probability that exactly n_{r_1} particles are contained in the cell centered about r_1 is

$$P(n_{r_1}) = \frac{1}{e} \frac{1}{n_{r_1}!} .$$

Then

$$\langle n_{r_1}^2 \rangle = \frac{1}{e} \sum_{n_{r_1}=0} \frac{n_{r_1}^2}{n_{r_1}!} = \frac{1}{e} \sum_{m=1} \frac{m}{(m-1)!}$$

$$= \frac{1}{e} \sum_{p=0} \frac{p+1}{p!} = \frac{1}{e} \left\{ \sum_{p=1} \frac{1}{(p-1)!} + \sum_{p=0} \frac{1}{p!} \right\}$$

$$= \frac{1}{e} \left\{ \sum_{q=0} \frac{1}{q!} + \sum_{p=0} \frac{1}{p!} \right\}$$

$$= \frac{2}{e} \sum_{q=0} \frac{1}{q!} = 2 .$$

With $< n_{r_1}^2 > = 2$ and reference to Equations (12), one can calculate $\langle V \rangle$ as follows:

$$\langle V \rangle = \frac{N\rho^2 U_o}{2} = \frac{N\rho^2}{2} \int U(r-r')d\tau\, d\tau' . \tag{15a}$$

For relatively short-range potentials, one can integrate over the volume τ' to obtain

$$\langle V \rangle = \frac{N\rho}{2} \int U(q)d\tau_q = \frac{N\rho}{2}\, g(0) \tag{15b}$$

where $q = |r-r'|$. The above result is identical with that obtained from first-order perturbation theory in the low-density region (59).

Next treat the case of free particles--that is, no interactions ($U_o=0$). The Hamiltonian in (14) becomes in this case

$$H = \frac{\hbar^2\rho^{\frac{2}{3}}}{m} \sum_{r_j} b^*_{r_j} b_{r_j} - \frac{\hbar^2\rho^{\frac{2}{3}}}{2m} \sum_{r_j} (b^*_{r_j} b_{r_j+r_o} + b^*_{r_j} b_{r_j-r_o}) . \tag{16}$$

A canonical transformation is made which diagonalizes the Hamiltonian--namely,

$$b_{r_j} = \frac{1}{\sqrt{N}} \sum_q a_q\, e^{iq\cdot r_j} . \tag{17}$$

Then

$$\sum_{r_j} b^*_{r_j} b_{r_j} = \frac{1}{N} \sum_{qsr_j} a^*_q a_s e^{ir_j \cdot (s-q)} = \sum_q a^*_q a_q$$

$$\sum_{r_j} b^*_{r_j} b_{r_j+r_o} = \frac{1}{N} \sum_{qsr_j} a^*_q a_s e^{ir_j \cdot (s-q)} e^{ir_o \cdot s} = \sum_q a^*_q a_q e^{ir_o \cdot q}$$

$$\sum_{r_j} b^*_{r_j} b_{r_j-r_o} = \frac{1}{N} \sum_{qsr_j} a^*_q a_s e^{ir_j \cdot (s-q)} e^{-ir_o \cdot s} = \sum_q a^*_q a_q e^{-ir_o \cdot q}$$

and Equation (16) reads

$$H = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} \sum_q a^*_q a_q (1 - \cos q \cdot r_o) \tag{18a}$$

$$= \sum_q \mathcal{E}_q \, a^*_q a_q \, . \tag{18b}$$

Since it follows from Equation (17) that a^*_q and a_q are creation and destruction operators, respectively, for plane waves of momentum q, $\mathcal{E}_q$ is the corresponding energy:

$$\mathcal{E}_q = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} (1 - \cos q \cdot r_o) \, . \tag{19}$$

For low momentum, corresponding to wavelengths long compared to the average distance between particles, expansion of the cosine function yields

$$\mathcal{E}_q = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} \left(\frac{1}{2} q^2 r_o^2\right) . \tag{20}$$

Since $\rho = \frac{1}{r_o^3}$,

$$\mathcal{E}_q = \frac{\hbar^2}{2m} q^2 , \tag{21}$$

a known result correct for free particles. It is noted that the appearance of the trigonometric function in Equation (19) is a direct consequence of the cell-type model which has here been employed.

Lastly, for low densities the Hamiltonian of Equation (14) can be approximated and subsequently diagonalized to yield the energy of low-momentum excitations which correspond to sound waves or phonons; the results agree with those of Brueckner and Sawada (60), Lee, Huang, and Yang (61), Bogoliubov (62), and others. One thus writes as a first approximation in this case

$$b_{r_j} = 1 + \xi_{r_j}$$

whereupon the Hamiltonian assumes the quadratic form†

$$H = \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \sum_{r_j} \left(2\xi^*_{r_j}\xi_{r_j} - \xi^*_{r_j}\xi_{r_j+r_o} - \xi^*_{r_j}\xi_{r_j-r_o}\right)$$

$$+ \frac{\rho^2 U_o}{2} N + \frac{\rho^2 U_o}{2} \sum_{r_j} \left(\xi^*_{r_j}\xi^*_{r_j} + 2\xi^*_{r_j}\xi_{r_j} + \xi_{r_j}\xi_{r_j}\right) . \tag{22}$$

---

†Details of the calculations involved in the present analysis are found in Appendix A.

As the ξ's are assumed to be small compared to unit, products of three or more of these quantities have been neglected. Introducing the plane wave representation

$$\xi_{r_j} = \frac{1}{\sqrt{N}} \sum_k a_k \, e^{ik \cdot r_j}$$

one finds that Equation (22) reads

$$H = \frac{N\rho^2 U_o}{2} + \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) a_k^* a_k + \frac{\rho^2 U_o}{2} \left(a_k^* a_{-k}^* + a_k a_{-k} \right) \right] . \tag{23}$$

The same approximation for low momentum has been used in obtaining (23) as was previously employed in arriving at Equation (21) from (19). To diagonalize the Hamiltonian of Equation (23) the following canonical transformation is introduced

$$a_k = u_k \eta_k + v_k \eta_{-k}^*$$

where $u_k^2 - v_k^2 = 1$ in order that the new operators may obey the same commutation rules as the old ones. With these commutation relations and the transformation cited, the Hamiltonian becomes (see Appendix A)

$$H = \frac{N\rho^2 U_o}{2} + \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) v_k^2 + \rho^2 U_o \, u_k \, v_k \right]$$

$$+ \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) \left(u_k^2 + v_k^2 \right) + 2\rho^2 U_o \, u_k \, v_k \right] \eta_k^* \eta_k +$$

$$+\sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o\right) u_k v_k + \frac{\rho^2 U_o}{2}\left(u_k^2 + v_k^2\right)\right]\left(\eta_k^* \eta_{-k}^* + \eta_k \eta_{-k}\right) .$$

That part of the Hamiltonian independent of operators is the ground state energy at low density, while the coefficient of $\eta_k^* \eta_k$ leads to the phonon spectrum. When the off-diagonal terms are equated to zero, the amplitudes u_k and v_k can be found, whereupon the energy E_k of the excited states assumes the well-known form

$$E_k = \left(\frac{\hbar^2 k^2}{2m}\right)^{1/2}\left(\frac{\hbar^2 k^2}{2m} + 2\rho^2 U_o\right)^{1/2} .$$

In conclusion, it is of interest to ponder the question of the quantum cell model and superfluid behavior. A criterion for superfluidity can be established by again transforming to plane wave representation. With the aid of Equation (17)

$$\langle b_{r_j}^* b_{r_k} \rangle = \frac{1}{N}\sum_{q,p} \langle a_q^* a_p \rangle e^{-iq\cdot r_j} e^{ip\cdot r_k}$$

or

$$\langle b_{r_j}^* b_{r_k} \rangle = \frac{1}{N}\sum_{q} \langle a_q^* a_q \rangle e^{-iq\cdot(r_j - r_k)} + \frac{1}{N}\sum_{q\neq p} \langle a_q^* a_p \rangle e^{-iq\cdot r_j} e^{ip\cdot r_k} .$$

The latter can be expanded to give

$$\langle b^{*}_{r_j} b_{r_k} \rangle = \frac{1}{N} \langle a^{*}_{o} a_{o} \rangle + \frac{1}{N} \sum_{q \neq o} \langle a^{*}_{q} a_{q} \rangle e^{-iq\cdot(r_j - r_k)}$$

$$+ \frac{1}{N} \sum_{q \neq p} \langle a^{*}_{q} a_{p} \rangle e^{-iq\cdot r_j} e^{ip\cdot r_k} .$$

For superfluidity in plane wave representation, a finite fraction of particles must be in the ground state (61)--that is, $\langle a^{*}_{o} a_{o} \rangle$ must be on the order of N, the total number of particles, irrespective of the exact form of the interparticle forces. Thus, from the above equation, $\lim_{|r_j - r_k| \to \infty} \langle b^{*}_{r_j} b_{r_k} \rangle$ will be finite, implying a long-range correlation between particles of the system. This criterion provides an interesting example of the duality between plane wave and cell occupation operators. It may be pointed out, however, that beginning for the dense system with a state in which there exists one particle per cell--a state fairly close to the actual ground state--the superfluid behavior will be exceedingly difficult to obtain. Although the off-diagonal terms in the kinetic energy will mix this initial state with other states describing multiply-occupied cells, a widespread wandering of particles must occur to establish adequate conditions for superfluidity. Nevertheless, the ground state energy should be determinable quite accurately since it is almost entirely dependent on local rather than long-range behavior within the system.

In this chapter, the Hamiltonian operator of Equation (14) has been derived on the basis of the cell model described at the outset. At

low densities, the Hamiltonian reproduces well-known results; in the case of close packing, the Hamiltonian appropriately tends to confine particles to their respective cells and thus prevents large-scale migration. Interest here centers predominantly on high-density Boson systems, and subsequent studies involve application of the Hamiltonian exclusively to such systems for a determination of certain ground state properties. Both one- and two-dimensional particle ensembles are investigated analytically.

CHAPTER III

PERTURBATION THEORY CALCULATION OF THE GROUND STATE ENERGY

It is the purpose in this chapter to compute the perturbed ground state energy of a dense system of Bose particles. The Hamiltonian of the system is that determined in Chapter II and presented in Equation (14). Digressing for a moment to the low density Bose system, one there characterizes the unperturbed ground state by the fact that all particles are in the free-particle zero-momentum state. Owing to the interaction, particles are excited from this state into various free-particle states of momentum unequal to zero. For the compact system, on the other hand, the unperturbed ground state is here taken as corresponding to one particle per cell in the cell-model representation outlined in Chapter II. Interactions between particles result in multiple occupancy of cells, but in view of the high density of the system only configurations of 0, 1, or 2 particles per cell are allowed in the perturbed ground state. Rayleigh-Schrödinger perturbation theory is employed to determine the energy correction ΔE which when added to the unperturbed ground state energy E_o yields the ground state energy E of the perturbed system

$$E = E_o + \Delta E \ . \tag{24a}$$

The Hamiltonian of Equation (14) is written as the sum of an unperturbed Hamiltonian H_o and a perturbed one H_1

$$H = H_o + H_1 \tag{24b}$$

where H_o constitutes the diagonal portion of the Hamiltonian

$$H_o = \frac{\hbar^2\rho^{\frac{2}{3}}}{m}\sum_j n_j + \frac{\rho^2 U_o}{2}\sum_j n_j(n_j - 1) \tag{25}$$

and

$$H_1 = -\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\sum_j b_j^* (b_{j+1} + b_{j-1}) . \tag{26}$$

The latter or off-diagonal part is regarded as a perturbation on H_o and involves the shift operators discussed in Chapter II. It is noted that a simplified notation has been introduced over that utilized earlier--namely, r_j is replaced by j and $r_j \pm r_o$ by $j \pm 1$. With one particle in a cell in the unperturbed ground state, the corresponding energy E_o of Equation (24a) is found with the aid of (25) to be

$$E_o = \langle H_o \rangle = N\frac{\hbar^2\rho^{\frac{2}{3}}}{m} . \tag{27}$$

DeWitt (63) has developed a very concise expression for the energy correction ΔE in the Rayleigh-Schrödinger perturbation theory, a result employed extensively by Brueckner (64) in his treatment of an electron gas and of nuclear structure, as well as in his discussions concerning a Bose system at low density. The reader is referred to Appendix B for

details on the development. According to DeWitt, the complete energy level shift is given by

$$\Delta E = \langle H_1 \rangle + \sum_{n=2}^{\infty} \sum_{\substack{k_i \geq 0 \\ k_1+k_2+\cdots+k_n=n-1}} (N_k+1)^{-1} \langle i | H_1 g_{k_1} H_1 \cdots g_{k_{n-1}} H_1 | i \rangle \qquad (28)$$

where $|i\rangle$ is the unperturbed ground state wave function and the coefficient involving N_k accounts for the cyclic rearrangements in any order which lead to the same result. Thus, N_k represents the number of indices k_i which, in any given arrangement, is equal to zero. The g's in Equation (28) are so-called propagators and are defined in terms of the projection operator $P_o^{(i)}$ on the i-th or unperturbed state:

$$g_o = - P_o^{(i)} \qquad (29)$$

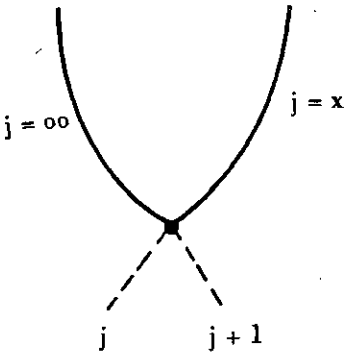
$$g_k = \frac{1 - P_o^{(i)}}{(H_o^{(i)} - H_o)^k} \qquad (k \geq 1) \qquad (30)$$

where the quantity in parentheses in the denominator of (30) is the energy of an intermediate state with respect to the unperturbed ground state as a basis. With the unperturbed ground state taken as corresponding to one particle per cell, one obtains for the first term in Equation (28)

$$\langle H_1 \rangle = 0 \ .$$

In the remainder of this chapter Equation (28) is used to calculate exactly the energy correction for a dense Boson system through the sixth order of perturbation theory. In addition, contributions to infinite order are determined for a particular class of excitations which constitutes the predominant part of the perturbed ground state energy. A graphical representation of the matrix elements in (28) is introduced to aid in future calculations and discussions. Thereby a single diagram presents a pictorial representation of a term in the perturbation expansion for the energy correction. A dashed line is to represent a particle in the chosen ground state, while a solid line denotes a particle in an intermediate state. The letter beside the line indicates the cell occupied by the corresponding particle, and a dot appears for each H_1 found in the matrix element. Each dot has exactly two lines joining it from below and exactly two lines proceeding upward from it. In any diagram the succession of events is arbitrarily chosen as upward, and the total number of dots is equal to the order of the perturbation. The pictorial representation described above is not to be taken as that of Feynman; however, a close correspondence to Brueckner diagrams (65) is noted. To demonstrate, the diagram in Figure 1 means the particles in cells j and j + 1 interact through H_1 resulting in a "hole" in cell j + 1 and a "double" (two particles) in cell j--that is, since H_1 is a shift operator, a particle is moved or shifted from one cell to a second cell immediately adjacent to the first.

A significant feature in evidence in Equation (28) is the appearance in every order of connected or linked diagrams as well as unlinked graphs. (The latter do not exist in second order.) Both linked and



oo : two particles in a cell

x : no particles in a cell

Figure 1. Pictorial Representation of the Interaction (Shift) of Single Particles in Cells j and j+1.

unlinked graphs contribute an amount to the energy correction which is proportional to N, the total number of particles. The unlinked diagrams, however, also contribute in proportion to powers of N higher than the first. It will be noted subsequently that, in fourth order, the unlinked terms of the latter type completely cancel one another, as indeed they do in sixth order. In fact, Goldstone (66) has shown that this cancellation of unlinked diagrams proportional to higher powers of N occurs in any order and is analogous to a cancellation of vacuum diagrams in field theory.

Two additional comments concerning Equation (28) are in order here. The perturbative operator H_1 shifts particles from cell to cell and the

matrix element in (28) is zero unless an even number of H_1's occur. An odd number of shifts will not return the system to the ground state. This means that all odd orders of the perturbation sequence are zero and only even orders need be considered. Furthermore, an unexcited intermediate state corresponds to a matrix element which is identically zero since the propagator in Equation (30) contains the projection operator in the form $(1 - P_o^{(1)})$.

Linked Contribution Through Sixth Order.--Figures 2 and 3 display, in the pictorial representation described earlier, the contributions to the matrix elements in (28) of all linked diagrams in second and fourth order ($n = 2, 4$), respectively. Figures 4, 5, and 6 depict those linked graphs contributing to the sixth order ($n = 6$) in the perturbation series, the former figure displaying only diagrams applicable when one single pair is found in an intermediate state. Since two pairs can also be formed in any intermediate state of sixth order--this is not possible in lower order--the set involving two pairs in but a single intermediate state is shown in Figure 5, while the graphs for two pairs in two intermediate states are contained in Figure 6. All of the diagrams depicted in Figures 2 through 6 have mirror-image counterparts which are not shown but must be accounted for in calculation of the energy correction. In addition, it is noted that although the displaced particle is regarded as originating in cell $j + 1$, cell $j - 1$ could just as well have been the origin, as evidenced by inspection of Equation (26). This fact is duly considered in the ultimate counting procedure involved in determining the energy.

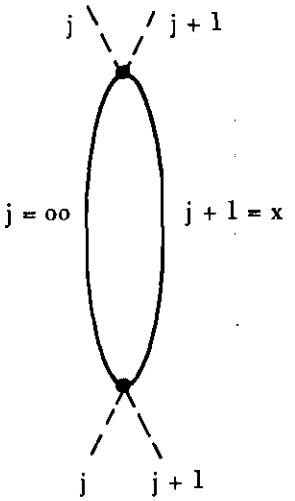


Figure 2. Linked Contribution to the Energy Correction in Second Order.

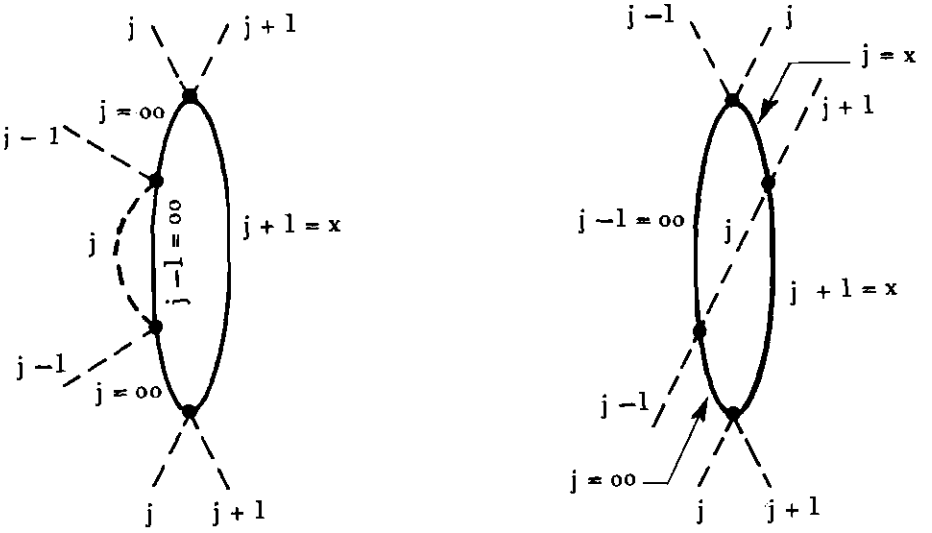


Figure 3. Linked Contributions to the Energy Correction in Fourth Order.

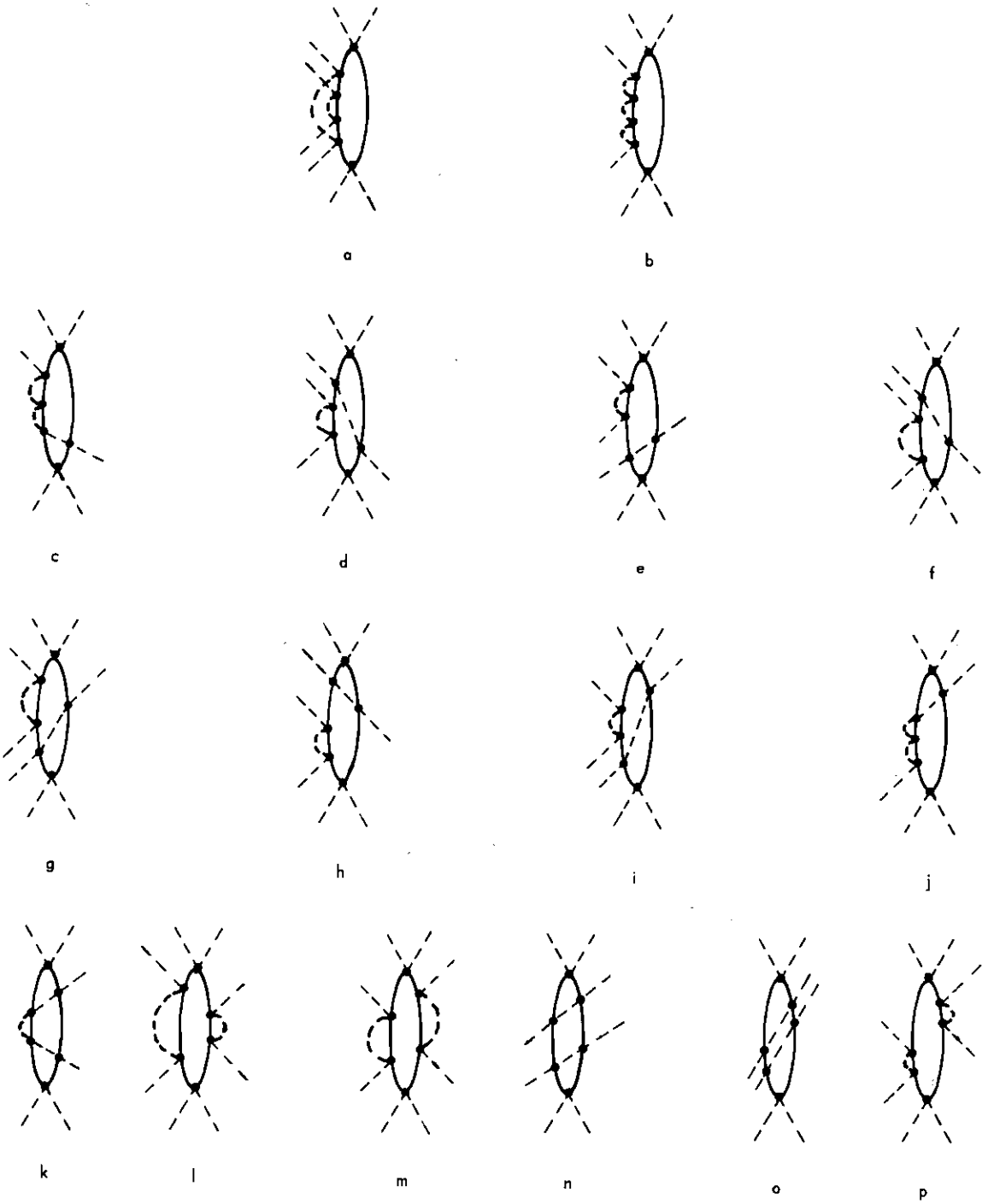


Figure 4. Linked Single Pair Contributions to the Energy Correction in Sixth Order.

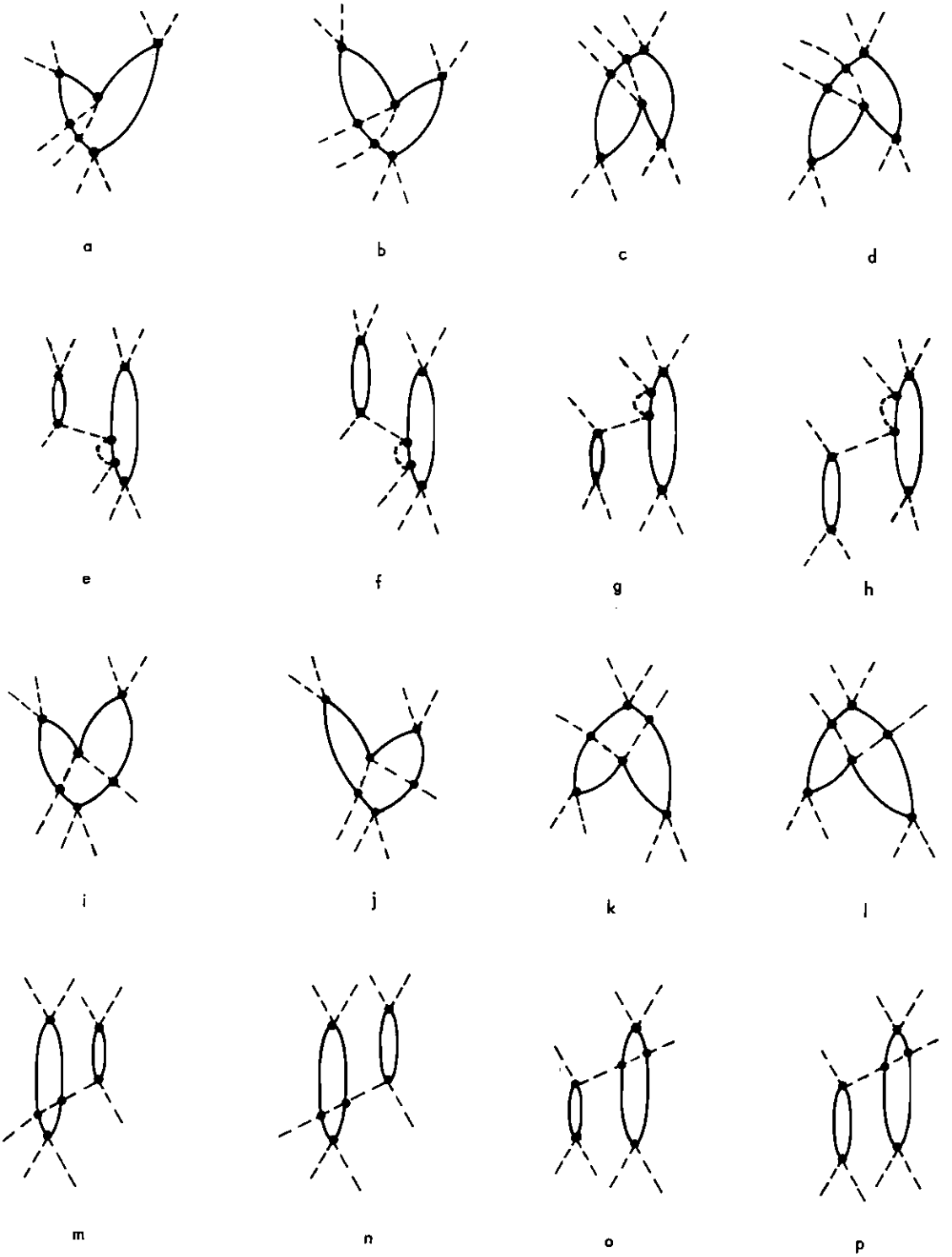


Figure 5. Linked Two Pair Contributions to the Energy Correction in Sixth Order.

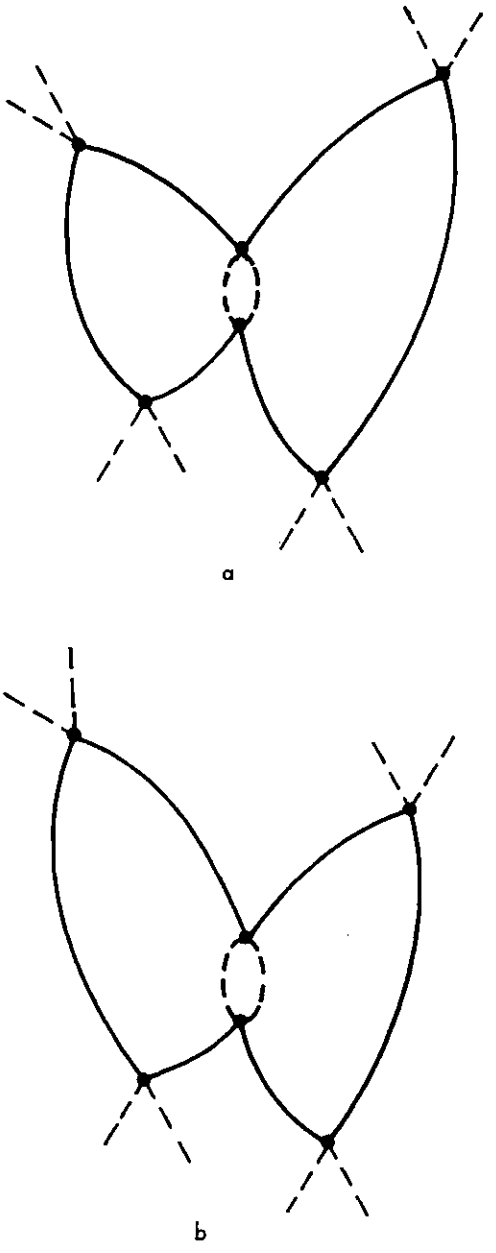


Figure 6. Additional Linked Two Pair Contributions to the Energy Correction in Sixth Order.

Figure 3a, with a "bubble" on the left side of the main loop, is indicative of a double propagating a unit cell distance; the mirror-image diagram represents the propagation of a hole for a unit distance through the cell structure. Figure 3b is interpreted as representing both a hole and a double propagating each a unit cell distance. In these and all ensuing diagrams, dots on the left side of a large loop denote propagation of a double, while dots on the right are for movements of the hole alone; each dot of the former type contributes a factor of 2 to the matrix element and each of the latter type a factor of unity. This occurs since the propagation of a double a unit cell distance involves the destruction of two and the creation of two particles. On the other hand, a hole propagating means the destruction of one and the creation of only one particle. Each vertex of a main loop (representing excitations from and to the unperturbed ground state) contributes an amount $\sqrt{2}$ since a particle is destroyed in one cell and two are created in an adjacent cell, or vice versa.

Existence of two pairs in one or more of the intermediate states, as in Figures 5 and 6, is easily recognized. In the event of single pairs alone (Figures 2, 3, and 4), any horizontal line drawn between successive dots across a given graph intersects but two solid lines. Should a horizontal line so drawn be found to intersect four solid lines, this means that two hole-double combinations exist at the corresponding intermediate level. This occurrence is evidenced at only one intermediate level in any of the representations depicted in Figure 5 and at two separate stages in each of the graphs of Figure 6.

The particular matrix elements of Equation (28) which refer to the linked diagrams in second, fourth, and sixth order are, respectively,

$$\langle i|H_1 g_1 H_1|i\rangle$$

$$\langle i|H_1 g_1 H_1 g_1 H_1 g_1 H_1|i\rangle$$

$$\langle i|H_1 g_1 H_1 g_1 H_1 g_1 H_1 g_1 H_1 g_1 H_1|i\rangle \ .$$

For single pairs alone, the energy denominator in the propagator of Equation (30) is simply $(-\rho^2 U_o)$ for all intermediate states with respect to the unperturbed ground state, a result immediately obtainable from Equation (25) with the imposed limitation on cell occupancy to a maximum of two particles for the dense system under consideration. For one intermediate state with two pairs, the relative energy is $(-2\rho^2 U_o)$, etc. Using the diagrams of Figures 2 through 6, one can write the linked contribution to the energy correction in second, fourth, and sixth order. Thus

$$(\Delta E)_2^{\ell} = -\,4N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^2 \frac{1}{\rho^2 U_o} = -\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x \qquad \text{(Figure 2)}$$

$$(\Delta E)_4^{\ell} = -\,36N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^4\left(\frac{1}{\rho^2 U_o}\right)^3 = -\,\frac{9}{4}\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x^3 \qquad \text{(Figure 3)}$$

$$(\Delta E)_6^{\ell,s} = -\,648\,N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5$$

$$= -\,\frac{81}{8}\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x^5 \qquad \text{(single pairs only; Figure 4)}$$

$$(\Delta E)_6^{\ell,m_1} = -\,432\,N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5$$

$$= -\,\frac{27}{4}\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x^5 \qquad \text{(one intermediate state with two pairs; Figure 5)}$$

$$(\Delta E)_6^{\ell,m_2} = -\,16\,N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5$$

$$= -\,\frac{1}{4}\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x^5 \qquad \text{(two intermediate states with two pairs; Figure 6)}$$

$$(\Delta E)_6^{\ell} = -\,1096\,N\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5$$

$$= -\,\frac{137}{8}\,N\,\frac{\hbar^2\rho^{\frac{2}{3}}}{m}\,x^5\,. \qquad \text{(total contribution)}$$

In the above, x represents the ratio of the kinetic energy of a particle localized in a cell to the effective potential energy for double occupancy and is given by

$$x = \frac{\hbar^2\rho^{\frac{2}{3}}/m}{\rho^2 U_o}\,. \tag{31}$$

It is noted that x is an expansion parameter in terms of which the perturbation series is developed. For the close packing (high density)

under study here, the quantity x is indeed small and thus constitutes a suitable parameter in which to express the ground state energy of the system. In a practical sense, x can be regarded as a measure of the system confinement, the smaller this parameter the less the particle wanderings or the greater the degree of locked-in behavior.

As a brief example of the calculations leading to the aforementioned energy corrections, consider $(\Delta E)_2^{\ell}$. Reference to Figure 2 reveals two main-loop vertices which contribute a factor $(\sqrt{2})^2$. Equation (26) specifies two separate operators and a summation over the N cells, hence a factor of 2N. Since but one diagram occurs in second order, the total contribution is 4N. In fourth order, four graphs occur--the two depicted in Figure 3 and their mirror images. Figure 3a contributes an amount $(\sqrt{2})^2(2)^2 = 8$; its mirror image $(\sqrt{2})^2(1)^2 = 2$. Figure 3b and its image contribute each the amount $(\sqrt{2})^2(2)^1(1)^1 = 4$. Thus the total contribution in fourth order is $2N(8 + 2 + 2 \times 4) = 36N$.

Unlinked Contribution Through Sixth Order.--The matrix elements which were cited in the previous subsection and which led to the linked contributions in second, fourth, and sixth order also yield unlinked contributions in these respective orders, with the exception of the second order. (No unlinked contribution to the energy shift is existent in the second order of perturbation.) Figures 7 through 9 contain pictorial representations of all unlinked contributions derivable from the matrix elements of the previous subsection. They represent processes in which hole-double combinations occur at two or three independent lattice locations with the subsequent propagation, in some cases, of the hole and/or

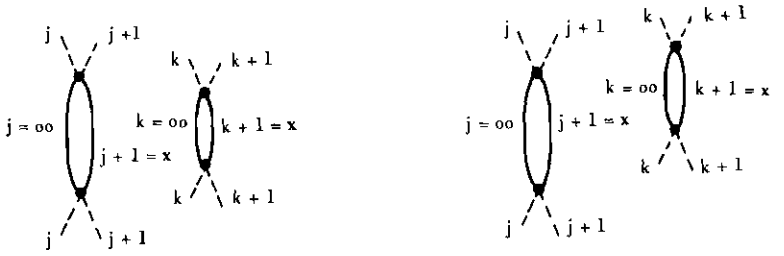


Figure 7. Unlinked Contributions to the Energy Correction in Fourth Order.

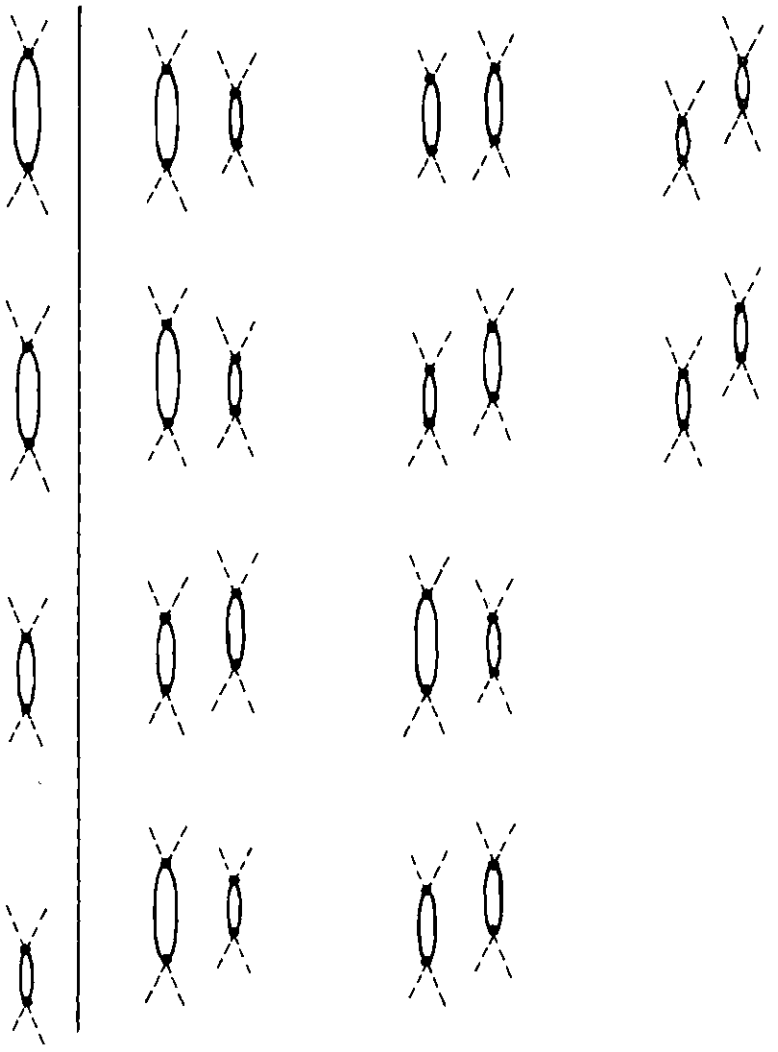


Figure 8. Unlinked Contributions Proportional to N(N-2)(N-4) for the Energy Correction in Sixth Order.

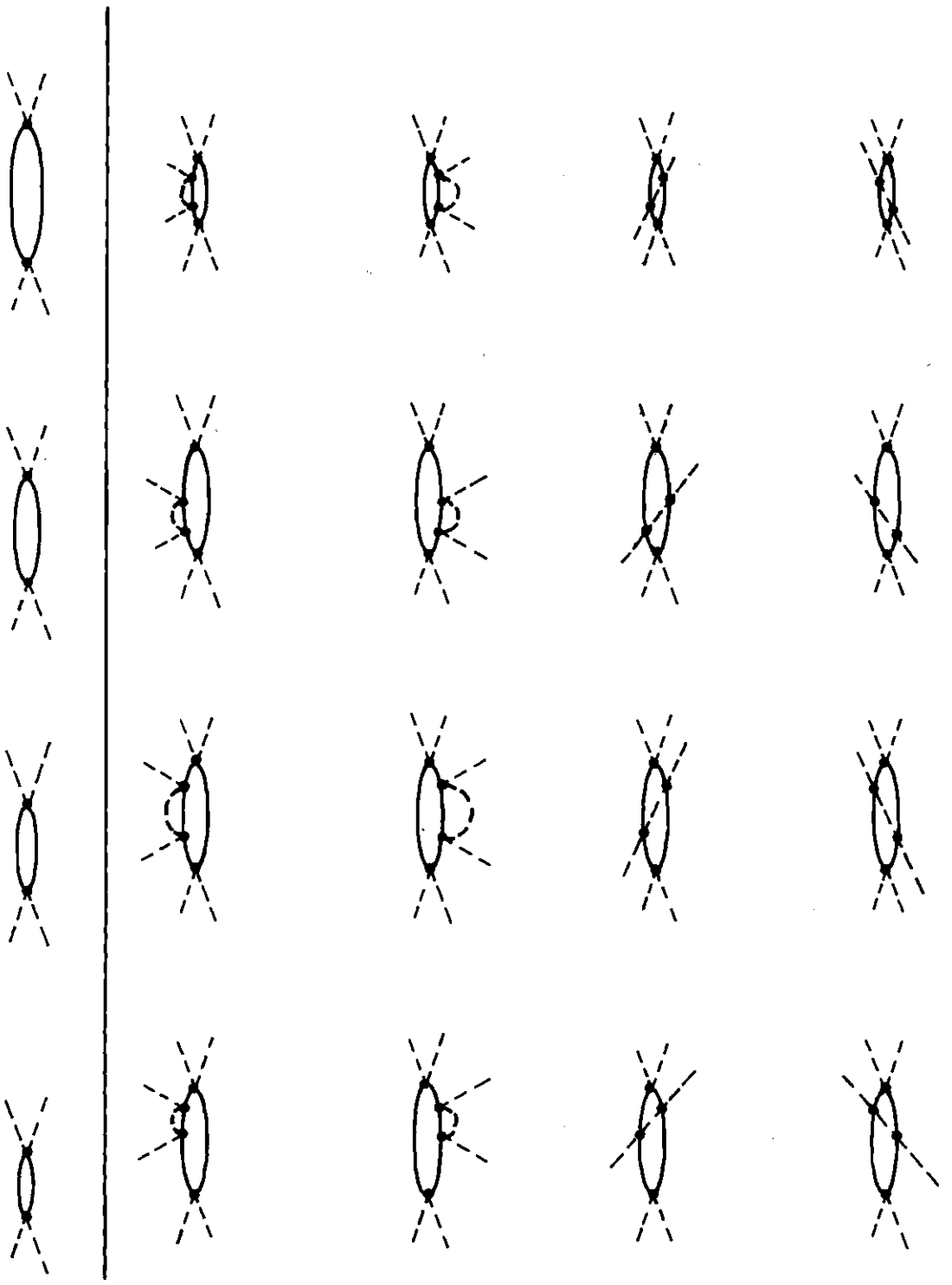


Figure 9a. Sixth Order Unlinked Contributions Proportional to N(N-2), Found by Combining Linked Fourth Order with Linked Second Order Diagrams.

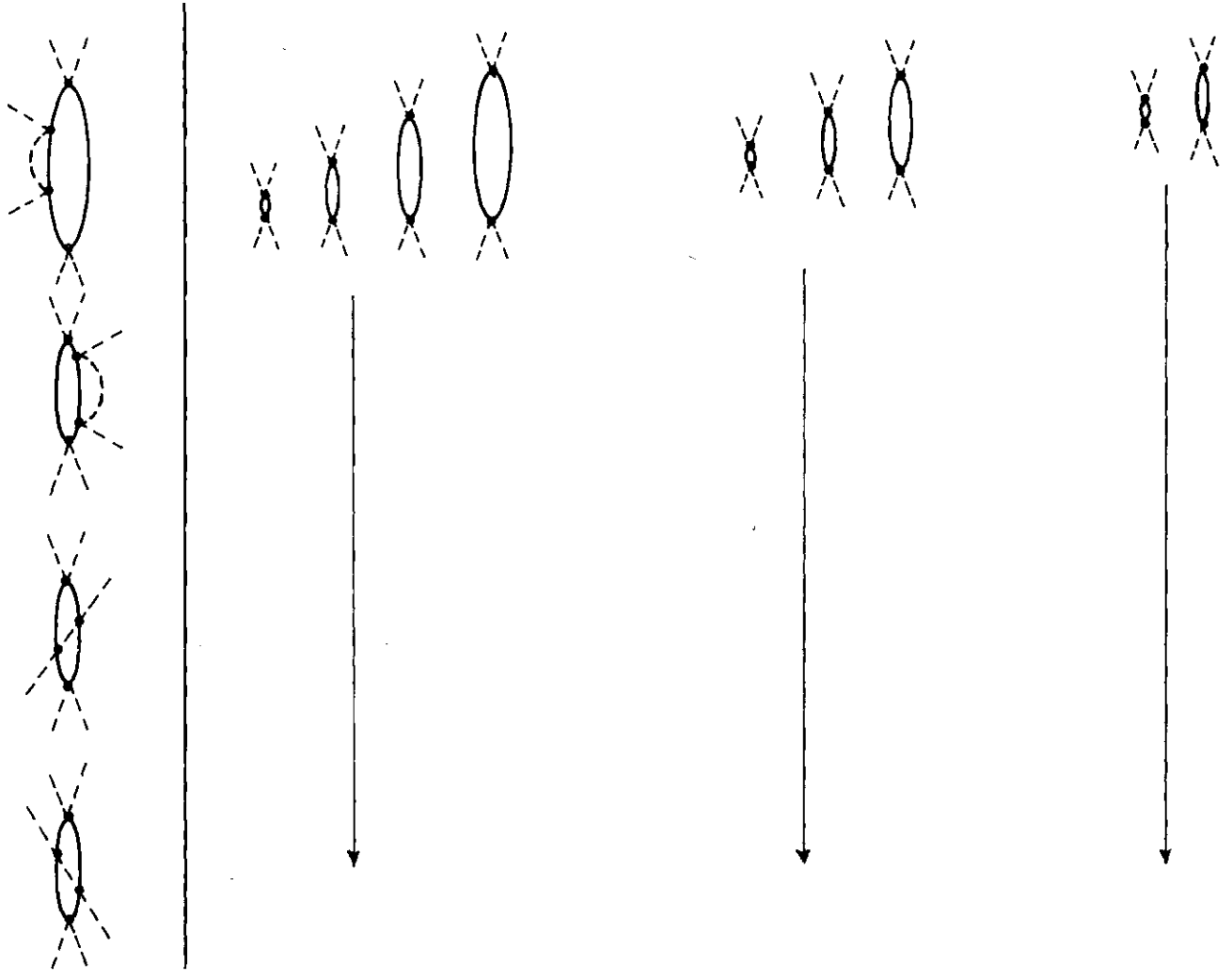


Figure 9b. Sixth Order Unlinked Contributions Proportional to N(N-2), Found by Combining Linked Second Order with Linked Fourth Order Diagrams.

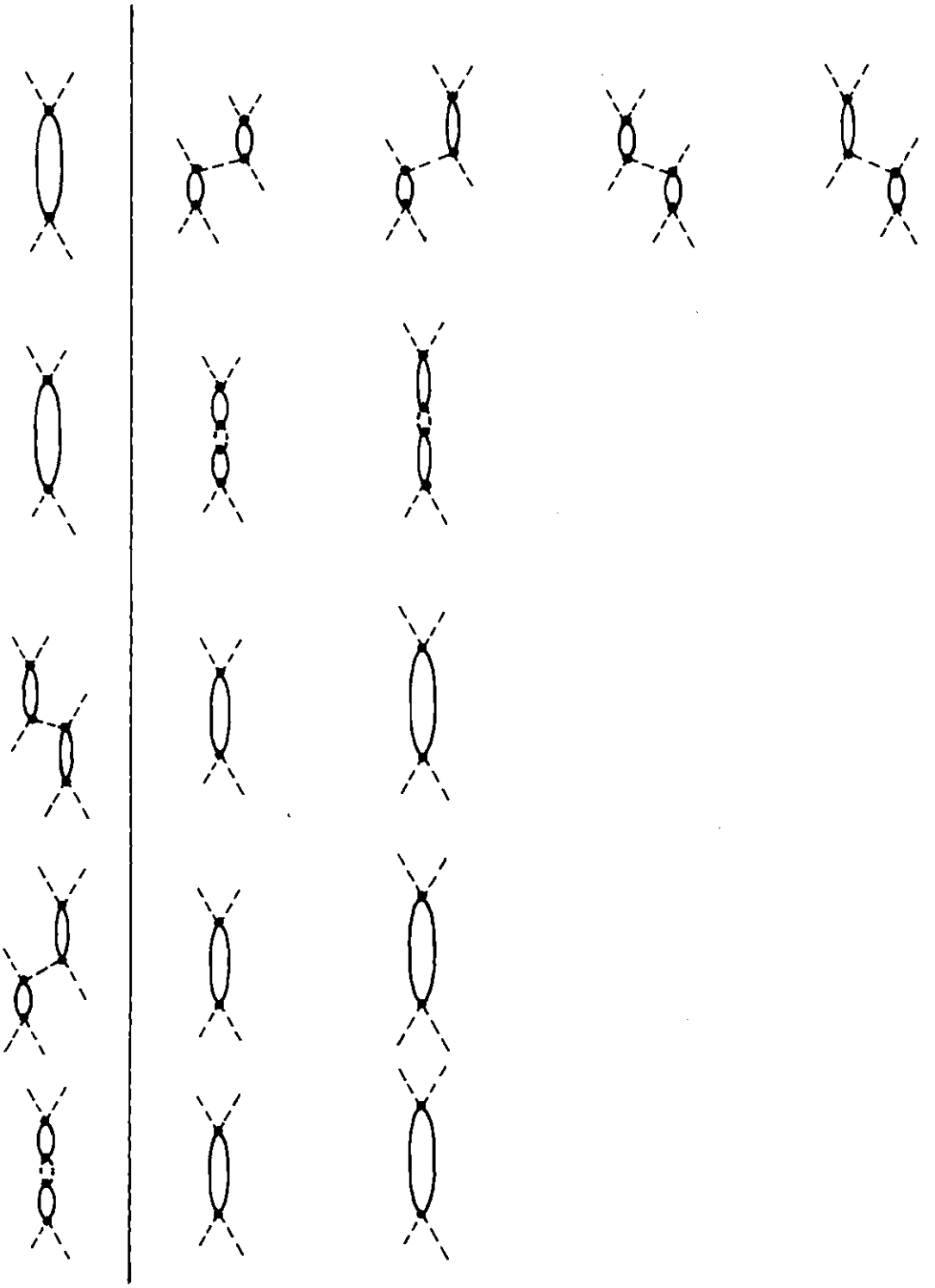


Figure 9c. Sixth Order Unlinked Contributions Proportional to N(N-2) and not Determined by Combinations of Linked Diagrams.

the double. For example, in each of the two distinct representations in Figure 7, one has a disconnected or unlinked graph in the obvious sense that j and k have no connection with one another. In field theory, similar unlinked diagrams are encountered--the so-called vacuum diagrams. The disconnected graphs of Figures 7 through 9 yield contributions to the energy shift in fourth and sixth order which are proportional to higher powers of the total particle number N, as well as contributing an energy correction proportional to N itself. The fact that contributions of order N arise here is clearly due to the depletion of the ground state. As noted earlier, in any given order a cancellation is realized of the contribution proportional to a power of N other than the first and arising from graphs such as those depicted in Figures 7, 8, and 9. This is brought about by the remaining terms found in Equation (28) which also pertain to the specified order. Such cancellations are presently displayed for the fourth and the sixth orders, and the net contribution proportional to N is recorded.

Figures 8 and 9 are to be interpreted as combinations of the diagram displayed on the left with a variety of graphs as shown on the right. Thus, in Figure 8, a second-order graph is seen to combine in many possible ways with fourth-order unlinked graphs of the type displayed in Figure 7. Since three independent primary loops occur, the contribution of the diagrams in Figure 8 are of the order $N(N-2)(N-4)$. Linked fourth order graphs are combined with linked second order graphs in Figure 9a, and linked second order with linked fourth order in all possible combinations in Figure 9b. The remaining unlinked contributions in sixth order are depicted in Figure 9c. All of the diagrams in Figure 9 contain

two primary loops representing two independent particles selected at random from the totality of N. These graphs therefore contribute in the order N(N-2) to the matrix elements of the previous subsection.

Statements of the foregoing subsection regarding the dots on the main loop apply as well in the case of the unlinked graphs. Care must be taken here to obtain the proper energy denominator in the propagator of Equation (30) since in some intermediate states only one pair exists while in others as many as three hole-double combinations are simultaneously in evidence. Furthermore, in any single unlinked diagram, each of the independent interaction graphs can occur in two different ways, corresponding to the double set of operators in Equation (26). With this in mind and with reference to Figures 7 through 9, one determines the unlinked contribution to the matrix elements already quoted in the previous subsection. There results:

Fourth Order: $$- 16N(N-2)\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^4\left(\frac{1}{\rho^2 U_o}\right)^3 \qquad \text{(Figure 7)}$$

Sixth Order: $$- 96N(N-2)(N-4)\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5 \qquad \text{(Figure 8)}$$

$$- 768N(N-2)\left(\frac{\hbar^2\rho^{\frac{2}{3}}}{2m}\right)^6\left(\frac{1}{\rho^2 U_o}\right)^5 \qquad \text{(Figure 9)}$$

The matrix element evaluated by means of Figure 7 leads to the contribution of $\frac{1}{2}(\sqrt{2})^4(2)4N(N-2)$, where the fourth power accounts for the four vertices of the two large loops, the factor of 2 the two diagrams, and $4N(N-2)$ the fact that two independent particles can each interact with their two respective neighbors and Equation (26) specifies a summation over all cells; the factor of 2 in the denominator occurs since there exists one intermediate state containing two pairs. Likewise, from Figure 8, one obtains $(\frac{1}{2})(\frac{1}{3})(\frac{1}{2})(\sqrt{2})^6(6)8N(N-2)(N-4)$ from those six diagrams which display two intermediate states with two doubles and one intermediate state of three pairs, and $(\frac{1}{2})(\frac{1}{2})(\sqrt{2})^6(4)8N(N-2)(N-4)$ from the four graphs which indicate two intermediate states of double pairs.

To show that, in each order, the contributions calculated above which are proportional to higher-than-first powers of N become nullified, it is necessary to consider the remaining matrix elements of Equation (28) in each order. In fourth order there is but one

$$- \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_2 H_1|i\rangle$$

which gives a contribution in N^2 of exactly the same magnitude but of opposite sign to that found from the unlinked graphs of Figure 7. Similarly, in sixth order the remaining matrix elements are

$$+ \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_3 H_1|i\rangle$$

$$- \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_1 H_1 g_1 H_1 g_2 H_1|i\rangle$$

$$- \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_1 H_1 g_2 H_1 g_1 H_1|i\rangle$$

$$- \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_2 H_1 g_1 H_1 g_1 H_1|i\rangle$$

$$+ \langle i|H_1 g_1 H_1|i\rangle \langle i|H_1 g_2 H_1|i\rangle \langle i|H_1 g_2 H_1|i\rangle$$

$$- \langle i|H_1 g_2 H_1|i\rangle \langle i|H_1 g_1 H_1 g_1 H_1 g_1 H_1|i\rangle$$

The contribution to the energy shift from each of these matrix elements is as follows:

$$+ \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \frac{1}{\rho^2 U_o} \right]^2 \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \left(\frac{1}{\rho^2 U_o} \right)^3 \right]$$

$$= - 64N^3 \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

$$- \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \frac{1}{\rho^2 U_o} \right] \left[36N + 16N(N-2) \right] \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^4 \left(\frac{1}{\rho^2 U_o} \right)^4$$

$$= (64N^3 + 16N^2) \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

$$- \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \frac{1}{\rho^2 U_o} \right] \left[36N + 8N^2 \right] \left(\frac{1}{\rho^2 U_o} \right)^5 \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^4 \left(\frac{1}{\rho^2 U_o} \right)^4$$

$$= (32N^3 + 144\ N^2) \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

$$- \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \frac{1}{\rho^2 U_o} \right] \left[36N + 16N(N-2) \right] \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^4 \left(\frac{1}{\rho^2 U_o} \right)^4$$

$$= (64N^3 + 16N^2) \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

$$+ \left[- 4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \frac{1}{\rho^2 U_o} \right] \left[4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \left(\frac{1}{\rho^2 U_o} \right)^2 \right]^2$$

$$= - 64N^3 \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

$$- \left[4N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^2 \left(\frac{1}{\rho^2 U_o} \right)^2 \right] \left[- 36N - 16N(N-2) \right] \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^4 \left(\frac{1}{\rho^2 U_o} \right)^4$$

$$= (64N^3 + 16N^2) \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5$$

By combining the results proportional to N^3 and to N^2 from the above with the respective values previously obtained from Figures 8 and 9, one obtains complete cancellation of all terms in higher powers of N. There remains then the unlinked contribution proportional to N. In fourth and sixth order, the energy shifts due to unlinked contributions proportional to N are:

$$(\Delta E)_4^u = 32N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right) \left(\frac{1}{\rho^2 U_o} \right)^3 = 2N \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} x^3$$

$$(\Delta E)_6^u = 768N \left(\frac{\hbar^2 \rho^{\frac{2}{3}}}{2m} \right)^6 \left(\frac{1}{\rho^2 U_o} \right)^5 = 12N \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} x^5 \ .$$

In the previous subsection the linked contribution through sixth order was established. With the calculation of the unlinked part of the energy correction through sixth order given above, one can combine the results to write for the total energy correction through sixth order

$$(\Delta E)_2 = - N \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} x$$

$$(\Delta E)_4 = - \frac{1}{4} N \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} x^3$$

$$(\Delta E)_6 = - \frac{41}{8} N \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} x^5 \ .$$

When the foresaid energy corrections are introduced into Equation (24a) together with the unperturbed energy E_o given by Equation (27), there follows the perturbed ground state energy per particle correct to sixth order for a system of dense Bosons based on the cell-model hypothesis of Chapter II:

$$\frac{E}{N} = \frac{\hbar^2 \rho^{\frac{2}{3}}}{m} \left(1 - x - \frac{1}{4} x^3 - \frac{41}{8} x^5 - - - \right) . \qquad (32)$$

A discussion of this function is postponed until Chapter VI, where it is compared with the ground state energy calculated by summing to infinite order the major contributors to the energy--namely, linked single pair excitations. This latter calculation follows.

Contribution of Linked Single Pair Excitations.--Since the major contribution in any order to the energy correction in Equation (28) is evidently realized from linked single pair excitations, it is the purpose here to

sum to infinite order all of the contributions from these excitations. The pictorial representations in Figures 2, 3, and 4 for the pertinent matrix elements in second, fourth, and sixth order of the perturbation series can be used to construct Table 1. This tabulation cites the amount of contribution to the energy correction from holes and doubles propagating in various permissible combinations of unit cell distances, all for single pair excitations only. A factor of $(-N\hbar^2\rho^{2/3}/m)$ has been deleted from each entry of Table 1. A slant line drawn in the table so as to connect terms of like power in x contains the entire contribution in a given order of perturbation, the order being higher by one than the exponent of x. Table 2 specifies which of the graphs in Figures 2, 3, and 4 have been taken into account in arriving at the numerical coefficients in Table 1. For example, the (1, 3) element in Table 1 reveals that eight separate diagrams apply when the double propagates three units and the hole but one unit. Table 2 lists these as Figures 4c through 4j. Primes in Table 2 refer to mirror-image graphs of those shown in Figures 2, 3, and 4.

Consider the total contribution to infinite order of the first column in Table 1--that is, the case in which the hole does not propagate while the double moves any even number of times, say $n(n \geq 0)$. The combinatorial numbers appearing in the first column (1, 1, 2, etc.) represent half the number of ways of starting at a given point on a one-dimensional periodic lattice and returning again after (n + 2) rectilinear steps (n = 0, 2, 4, etc.), with no prior returns permissible. This fact becomes evident from an inspection of the relevant matrix elements of Equation (28) and Figures 2, 3, and 4. After a double has

Table 1. Energy Contribution for Various Hole-Double Propagations

Double Moves \ Hole Moves	0	1	2	3	4
0	$1\ x$		$1\ \frac{1}{2^2}\ x^3$		$2\ \frac{1}{2^4}\ x^5$
1		$2\ \frac{1}{2}\ x^3$		$8\ \frac{1}{2^3}\ x^3$	
2	$1\ x^3$		$12\ \frac{1}{2^2}\ x^5$		
3		$8\ \frac{1}{2}\ x^5$			
4	$2\ x^5$				

Table 2. Reference Diagrams for Table 1

Double Moves \ Hole Moves	0	1	2	3	4
0	Figure 2		3a'		4a', 4b'
1		3b, 3b'		4c' to 4j'	
2	3a		4k to 4p 4k' to 4p'		
3		4c to 4j			
4	4a, 4b				

propagated n times, it must again occupy its original position in order to interact with the hole and return the system to the ground state. Because of the presence of the projection operator in a matrix element, any interaction of the double with the hole at an intermediate state leads to zero contribution for the matrix element; hence the condition disallowing intermediate returns to the origin. One thus encounters in the determination of the combinatorial numbers a one-dimensional restricted random-walk problem.

Chandrasekhar (67) has solved a one-dimensional random walk problem involving an absorbing barrier; he derives the number of ways $C(M,P,M_1)$ of arriving at M from the origin after P steps with absorber at M_1 in the form

$$C(M,P,M_1) = \binom{P}{\frac{1}{2}(P+M)} - \binom{P}{\frac{1}{2}(P+M) - M_1} \qquad (33)$$

where the right side is written in the familiar notation of binomial coefficients. To apply this result in order to determine an expression giving the entire array of combinatorial numbers in the first column of Table 1, one first imagines that one of the (n+2) total steps has occurred. This position, one removed from the original lattice point, becomes the origin; the absorber is placed at the original lattice position to insure that no intermediate returns can occur. Of the (n+1) remaining steps, then, n are available for the double to propagate outward and return to the established origin. In the symbology of Equation (33), P = n, M = 0, $M_1 = -1$. Therefore, from (33),

$$C(0,n,-1) = \frac{2}{n+2}\binom{n}{n/2} \equiv C(n) \tag{34}$$

gives the desired combinatorial numbers.

Once the appropriate combinatorial expression for the entries in the second column of Table 1 has been ascertained, it will be a simple matter to establish the general combinatorial law for the entire hierarchy in Table 1 and thereby evaluate the total contribution of linked single pairs. Centering one's interest now on the second column, wherein the hole propagates one unit cell distance while the double propagates any odd number m of units ($m \geq 1$), one can express the combinatorial numbers which appear in terms of a number of one-dimensional restricted random walk problems. Since the hole can "make its move" before or after the double has propagated m units, or indeed following any step which the double takes, it is necessary to study each possibility. Thus one considers first the double as propagating one unit distance, then three, then five, etc. At any stage, the hole is allowed to propagate one unit. For example, if the double propagates but one unit ($m = 1$), two possibilities exist--namely, the double moves one unit and the hole follows or the hole propagates one unit and the double follows. This is represented by the factor of 2 in the first entry, second column, of Table 1. If the double propagates three units ($m = 3$), eight possibilities exist corresponding to: hole moves first and double follows making three steps; double moves once, then hole moves once, then double moves twice more; double moves twice, then hole moves once, then double moves one more step; and, finally, double moves three times, then hole moves once.

Table 3. Data for a Series of Random Walk Problems

m	M	P	M_1	x	M	P	M_1
1	-1	1	-2		1	1	-1
	1	1	-1		1	1	-1
3	-1	3	-2		1	1	-1
	1	3	-1		1	1	-1
	0	2	-1		1	1	-1
	-2	2	-3		1	1	-1
	-1	1	-2		0 2	2	-1
5	-1	5	-2		1	1	-1
	1	5	-1		1	1	-1
	0	4	-1		1	1	-1
	-2	4	-3		1	1	-1
	-1	3	-2		0 2	2	-1
	-3	3	-4		2	2	-1
	0	2	-1		1	3	-1
	-2	2	-3		1 3	3	-1
	-1	1	-2		0 2	4	-1

In studying the process described above for several values of m, it becomes apparent that for each value of m the total possibilities involved can be expressed as the sum of several random walk problems. Table 3 summarizes the procedure for m = 1, 3, 5, where the notation of Equation (33) is employed. Thus, for m = 1 the combinatorial number is

$$C(-1, 1, -2)\, C(1, 1, -1) + C(1, 1, -1)\, C(1, 1, -1)$$

while for m = 3 it is given by the sum

$$C(-1, 3, -2)\, C(1, 1, -1) + C(1, 3, -1)\, C(1, 1, -1)$$

$$+ C(0, 2, -1)\, C(1, 1, -1) + C(-2, 2, -3)\, C(1, 1, -1)$$

$$+ C(-1, 1, -2)\, [C(0, 2, -1) + C(2, 2, -1)] .$$

Close examination of Table 3 and the overall problem itself reveals that, for any m, the desired combinatorial expression can be written as the sum of the following groups of terms, each group being contained within a set of parentheses:

$$\{C(-1, m, -2)\, C(1, 1, -1)\}$$

$$+ \{C(0, m-1, -1)\, C(1, 1, -1)$$
$$+ C(-2, m-1, -3)\, C(1, 1, -1)\}$$

$$+ \{C(-1, m-2, -2)\, [C(0, 2, -1) + C(2, 2, -1)]$$
$$+ C(-3, m-2, -4)\, C(2, 2, -1)\}$$

$$+ \{C(0, m-3, -1)\ C(1, 3, -1)$$
$$+ C(-2, m-3, -3)\ [C(1, 3, -1) + C(3, 3, -1)]$$
$$+ C(-4, m-3, -5)\ C(3, 3, -1)\}$$

$$+ - - -$$
$$\vdots$$
$$+ \{C(-1, 1, -1)\ [C(0, m-1, -1) + C(2, m-1, -1)]\}$$

$$+ \{C(1, m, -1)\ C(1, 1, -1)\} \ . \qquad (35)$$

There are (m+1) groups in the above expression, each of which has an identical sum. Using Equation (33), one obtains immediately the value of the first and the last groups--namely,

$$C(-1, m, -2)\ C(1, 1, -1) = C(1, m, -1)\ C(1, 1, -1) = C(m+1)$$

where C(n) is defined in Equation (34). Similarly, one finds that the second, third, etc. group each has the value C(m+1). That this is true for the general or q-th group is established in Appendix C.

The combinatorial expression which specifies the numerical coefficients in the second column of Table 1 is therefore

$$(m+1)\ C(m+1)$$

where m is the (odd) number of units that the double propagates in the lattice while the hole propagates but one unit. Previously it was found that when the hole does not propagate and the double propagates n(even) units, the relevant combinatorial expression is C(n). Defining

p = number of hole propagations

q = number of double propagations

and noting the symmetry apparent in Table 1, one can write the combinatorial factor F(p, q) for any term (p, q) in Table 1 and thus for any term in the perturbation series for linked single pairs--namely

$$F(p,\ q) = \frac{(p+q)!}{p!\ q!}\ C(p+q) \tag{36}$$

where C(n) is defined in (34). This is merely the product of two terms the first of which expresses the number of ways in which (p + q) objects may be arranged in two groups of, respectively, p and q objects each. The second term of the product is half the number of ways of starting at a given point on a one-dimensional periodic lattice and returning again after (p + q) rectilinear steps, excluding intermediate returns.

One now proceeds to sum to infinite order, column by column, the energy correction terms of Table 1. Thus

$$\frac{(\Delta E)^{\ell,s}}{-N\frac{\hbar^2\rho^{2/3}}{m}} = \sum_{\substack{q=0\\ q\ \text{even}}} F(0,\ q)\ x^{q+1} + \frac{1}{2}\sum_{\substack{q=1\\ q\ \text{odd}}} F(1,\ q)\ x^{q+2}$$

$$+ \frac{1}{2^2}\sum_{\substack{q=0\\ q\ \text{even}}} F(2,\ q)\ x^{q+3} + \frac{1}{2^3}\sum_{\substack{q=1\\ q\ \text{odd}}} F(3,\ q)\ x^{q+4}$$

$$+ \frac{1}{2^4}\sum_{\substack{q=0\\ q\ \text{even}}} F(4,\ q)\ x^{q+5} + - - - \tag{37}$$

where $(\Delta E)^{\ell,s}$ designates the entire energy correction for linked single pairs. Each of the terms appearing above can be expressed in an alternate manner. For example, with the aid of Equation (36),

$$\sum_{\substack{q=0 \\ q \text{ even}}} F(0, q)\, x^{q+1} = \sum_{\substack{q=0 \\ q \text{ even}}} C(q)\, x^{q+1} = \frac{1}{x} \sum_{\substack{p=2 \\ p \text{ even}}} C(p-2)\, x^{p}$$

$$\sum_{\substack{q=1 \\ q \text{ odd}}} F(1, q)\, x^{q+2} = \sum_{\substack{q=1 \\ q \text{ odd}}} (q+1)\, C(q+1)\, x^{q+2} = \frac{1}{x} \sum_{\substack{p=2 \\ p \text{ even}}} (p-2)\, C(p-2)\, x^{p}$$

$$\sum_{\substack{q=0 \\ q \text{ even}}} F(2, q)\, x^{q+3} = \sum_{\substack{q=0 \\ q \text{ even}}} \frac{(q+1)(q+2)}{2!}\, C(q+2)\, x^{q+3}$$

$$= \frac{1}{x} \sum_{\substack{p=2 \\ p \text{ even}}} \frac{(p-2)(p-3)}{2!}\, C(p-2)\, x^{p}$$

$$\sum_{\substack{q=1 \\ q \text{ odd}}} F(3, q)\, x^{q+4} = \sum_{\substack{q=1 \\ q \text{ odd}}} \frac{(q+1)(q+2)(q+3)}{3!}\, C(q+3)\, x^{q+4}$$

$$= \frac{1}{x} \sum_{\substack{p=2 \\ p \text{ even}}} \frac{(p-2)(p-3)(p-4)}{3!}\, C(p-2)\, x^{p} .$$

Equation (37) therefore takes the form

$$x \frac{(\Delta E)^{\ell,s}}{-N\frac{\hbar^2\rho^{2/3}}{m}} = \sum_{\substack{p=2\\ p\ \text{even}}} \left\{1 + \frac{1}{2}(p-2) + \frac{1}{2^2}\frac{(p-2)(p-3)}{2!}\right.$$

$$\left. + \frac{1}{2^3}\frac{(p-2)(p-3)(p-4)}{3!} + - -\right\} C(p-2)\, x^p \,. \tag{38}$$

The quantity in the braces in (38) is recognized as the Binomial Expansion of $(1 + \frac{1}{2})^{p-2}$, or $\frac{4}{9}(\frac{3}{2})^p$. Consequently, Equation (38) reads

$$\frac{9x}{4} \frac{(\Delta E)^{\ell,s}}{-N\frac{\hbar^2\rho^{2/3}}{m}} = \sum_{\substack{p=2\\ p\ \text{even}}} C(p-2)\, X^p \tag{39}$$

where

$$X = \frac{3}{2}x \,. \tag{40}$$

Next, the right member of (39) is evaluated. With

$$S = \sum_{\substack{p=2\\ p\ \text{even}}} C(p-2)\, X^p = \sum_{\substack{p=2\\ p\ \text{even}}} \frac{2}{p}\binom{p-2}{\frac{p}{2}-1} X^p \tag{41}$$

found by introducing Equation (34), one can write

$$S = \sum_{s=1} \frac{1}{s}\binom{2s-2}{s-1} X^{2s} \,. \tag{42}$$

Since $\binom{2s-2}{s-1}$ is the coefficient of y^{s-1} in the expansion of $(1+y)^{2s-2}$ in a Laurent series, the following is valid (68)

$$\binom{2s-2}{s-1} = \frac{1}{2\pi i} \oint \frac{dy}{y^s} \left(1 + y\right)^{2s-2} . \tag{43}$$

Also

$$\frac{X^{2s}}{s} = 2\int_0^X z^{2s-1}\, dz . \tag{44}$$

Therefore, Equation (42) can be expressed in the equivalent form

$$S = \frac{1}{\pi i} \oint \frac{dy}{(1+y)^2} \int_0^X \frac{dz}{z} \sum_{p=1}^{\infty} \left[\frac{(1+y)^2}{y} z^2 \right]^p$$

$$= \frac{1}{\pi i} \oint \frac{dy}{y} \int_0^X z\, dz \left[\frac{1}{1 - \frac{z^2(1+y)^2}{y}} \right] . \tag{45}$$

With the introduction of the substitution $y = e^{i\phi}$, the above expression simplifies to

$$S = \frac{2}{\pi} \int_0^X z\, dz \int_0^{\pi} \frac{d\phi}{1 - 2z^2(1 + \cos\phi)}$$

$$= 2\int_0^X \frac{z\, dz}{\sqrt{1 - 4z^2}}$$

$$= \frac{1}{2}\left[1 - \sqrt{1 - 4X^2} \right] . \tag{46}$$

Equation (39) for the energy correction appertaining in the case of linked single pair excitations becomes, in view of Equations (40) and (46),

$$(\Delta E)^{\ell,s} = - N \frac{\hbar^2 \rho^{2/3}}{m} \frac{2}{9x} \left(1 - \sqrt{1 - 9x^2}\right) . \qquad (47)$$

By expanding the square root one has

$$(\Delta E)^{\ell,s} = - N \frac{\hbar^2 \rho^{2/3}}{m} \left(x + \frac{9}{4} x^3 + \frac{81}{8} x^5 + - - - \right)$$

which agrees exactly with the linked contribution through sixth order as calculated earlier. Finally, Equation (47), together with (27), is substituted into (24a) to obtain the perturbed ground state energy per particle when only linked single pair excitations are considered:

$$\frac{E^{\ell,s}}{N} = \frac{\hbar^2 \rho^{2/3}}{m} \left[1 - \frac{2}{9x} \left(1 - \sqrt{1 - 9x^2}\right)\right] . \qquad (48)$$

This represents a monotonic function of the expansion parameter x, defined in Equation (31), within the limits of definition--that is, for $x \leq \frac{1}{3}$. A plot and a discussion of (48) is contained in Chapter VI.

Modification of the Propagator.--In order to accommodate the contribution to the energy correction which is proportional to N and which arises by virtue of unlinked graphs such as those depicted in Figures 7 through 9, the propagator of Equation (30) can be modified. With the new propagator and the linked diagrams only, both the linked and the unlinked contributions previously determined separately should be

realized from a single calculation. The unmodified propagator of Equation (30) is designated by $\frac{1}{b_o}$, where

$$\frac{1}{b_o} = \frac{1}{-\rho^2 U_o} \quad . \tag{49}$$

Writing $\frac{1}{b}$ for the modified propagator, one expresses it in a form analogous to that introduced by Brueckner (64)--namely,

$$\frac{1}{b} = \frac{1}{-\rho^2 U_o + 2\langle K \rangle} \tag{50}$$

in which the operator K is given by

$$K = v_{j\pm1,j} + v_{j,j\pm1} \frac{1}{b} K \tag{51}$$

and $v_{j,j\pm1}$ represents a localized perturbation operator--that is, it expresses the incremental change in kinetic energy as a particle shifts from cell j to an adjacent cell $j\pm1$:

$$v_{j,j\pm1} = -\frac{\hbar^2 \rho^{2/3}}{2m} \left[b_j^* (b_{j+1} + b_{j-1}) \right] . \tag{52}$$

The above quantity thus constitutes a single term in the perturbed Hamiltonian operator given by Equation (26). Similarly,

$$v_{j\pm1,j} = -\frac{\hbar^2 \rho^{2/3}}{2m} \left[(b_{j+1}^* + b_{j-1}^*) b_j \right]$$

and represents shifts from cell $j\pm1$ to j.

Consideration is now given only nearest-neighbor hole-double pairs; thus the modified propagator of Equation (50), when used to calculate the energy correction, should yield in this approximation the contribution of the terms shown graphically in Figures 2 and 7 above. The operator equation for K is to be solved in first approximation and the result introduced into (50). Hence

$$(1 - v_{j,j\pm1}\frac{1}{b})K = v_{j\pm1,j}$$

or

$$K = \frac{v_{j\pm1,j}}{1 - v_{j,j\pm1}\frac{1}{b}}$$

$$= \frac{v_{j\pm1,j}}{1 - v_{j,j\pm1}\frac{1}{-\rho^2 U_o + 2\langle K\rangle}} \tag{53}$$

where the latter results by virtue of Equation (50). Equation (53) is expressible as an infinite sum

$$K = v_{j\pm1,j}\sum_{n=0}^{\infty}\frac{(v_{j,j\pm1})^n}{(-\rho^2 U_o + 2\langle K\rangle)^n}$$

whereupon the expectation value of K becomes

$$\langle K \rangle = \langle v_{j\pm1,j} \rangle + \frac{\langle v_{j\pm1,j}\ v_{j,j\pm1} \rangle}{-\rho^2 U_o + 2\langle K \rangle} \tag{54}$$

since hole-double pairs exist at nearest-neighbor distance only.

Equation (54) can now be solved for $\langle K \rangle$ and the result introduced into (50) to give the new propagator. The matrix element $\langle v_{j\pm1,j}\ v_{j,j\pm1} \rangle$ represents a closed loop of the type shown in Figure 2 and thus has the value

$$\langle v_{j\pm1,j}\ v_{j,j\pm1} \rangle = 2\left(-\frac{\hbar^2\rho^{2/3}}{2m}\right)^2 \left(\sqrt{2}\right)^2$$

$$= \left(\frac{\hbar^2\rho^{2/3}}{m}\right)^2 .$$

Equation (54) then assumes the quadratic form

$$\langle K \rangle^2 - \frac{\rho^2 U_o}{2}\langle K \rangle - \frac{1}{2}\left(\frac{\hbar^2\rho^{2/3}}{m}\right) = 0$$

whereupon

$$\langle K \rangle = \frac{\rho^2 U_o}{4}\left[1 - (1 + 8x^2)^{1/2}\right] . \tag{55}$$

The parameter x appearing in (55) has been defined earlier in Equation (31). Introduction of (55) into (50) leads to the modified propagator

$$\frac{1}{b} = \frac{1}{-\frac{\rho^2 U_o}{2}\left[1 + (1 + 8x^2)^{1/2}\right]} . \tag{56}$$

The second-order energy correction can now be found with the aid of the modified propagator. From Equation (28)

$$(\Delta E)_2^{\ell,u} = \langle H_1 \frac{1}{b} H_1 \rangle \tag{57}$$

where H_1 and $\frac{1}{b}$ are given by Equations (26) and (56), respectively, and the matrix element includes the second-order linked contribution and the fourth-order unlinked contribution proportional to N. Thus, Equation (57) leads to

$$(\Delta E)_2^{\ell,u} = N\left(\frac{\hbar^2\rho^{2/3}}{m}\right)^2 \frac{1}{-\rho^2 U_o\left[1 + (1 + 8x^2)^{1/2}\right]}$$

$$= -2N \frac{\hbar^2\rho^{2/3}}{m} \frac{x}{1 + (1 + 8x^2)^{1/2}} \tag{58a}$$

$$= N \frac{\hbar^2\rho^{2/3}}{m} \frac{1}{4x}\left[1 - (1 + 8x^2)^{1/2}\right]. \tag{58b}$$

A binomial expansion of Equation (58b) through two terms yields

$$(\Delta E)_2^{\ell,u} = -N \frac{\hbar^2\rho^{2/3}}{m} x + 2N \frac{\hbar^2\rho^{2/3}}{m} x^3 \tag{59}$$

in which the first term is the second-order linked contribution as previously obtained from Figure 2, and the second term is the total fourth-order unlinked result calculated earlier by means of Figure 7.

A few interesting sidelights may be derived from the foregoing analysis. From Equation (56) the effective energy E_{eff} of a hole-double

pair at nearest-neighbor distance can be stipulated in the limits of the approximation here made:

$$E_{eff} = \frac{\rho^2 U_o}{2}\left[1 + (1 + 8x^2)^{1/2}\right] . \qquad (60)$$

In addition, it is noted that the energy correction for but a single nearest-neighbor pair is the first term in Equation (59), while that for many pairs is given by (58b). The ratio of the two may be used as a measure of the number N_o of singly-occupied cells:

$$\frac{N_o}{N} = \frac{2}{1 + (1 + 8x^2)^{1/2}} . \qquad (61)$$

As one would anticipate, at very high density ($x \to 0$) all of the cells tend to be singly occupied, while the effective energy of formation for a hole-double combination is very large--namely, $\rho^2 U_o$. For increasing x, more and more hole-double pairs are formed and E_{eff} in (60) increases. This means that as more and more pairs form, the energy to excite another pair becomes larger and larger making each subsequent pair formation the less likely to occur.

In review, Chapter III includes a calculation of the ground state energy for a dense Boson system predicated upon the quantum cell model described in Chapter II. Rayleigh-Schrödinger perturbation theory was employed throughout, and the energy was determined exactly through the sixth order. This involved linked and unlinked contributions, the former including single and multiple pair excitations. Furthermore, the energy contribution arising from the entire set of linked single pair interactions

was established by analogy with one-dimensional restricted random walk problems. This latter procedure proves exceptionally advantageous in the case of a two-dimensional particle array as outlined in Chapter V. Modification of the propagator in order to lump linked and unlinked contributions has been achieved at least through the fourth order of unlinked terms. In the following chapter, the ground state wave function descriptive of nearest-neighbor hole-double combinations is discussed, and the Schrödinger equation is solved to obtain the selfsame energy contribution from hole-double pairs at nearest-neighbor distance as was obtained in the present chapter by means of the propagator modification.

CHAPTER IV

GROUND STATE WAVE FUNCTION FOR NEAREST-NEIGHBOR HOLE-DOUBLE PAIRS

Although the complete ground state wave function of the Hamiltonian given in Equation (14) of Chapter II has not been ascertained, the wave function ψ_o when nearest-neighbor hole-double pairs only are considered has been established. With ψ_o written in terms of "pair occupation" states, it is here displayed that this wave function when introduced with the Hamiltonian into the Schrödinger equation yields the ground state energy already found in the previous chapter. Designating by ℓ_o the number of particles not involved in a hole-double combination and by ℓ the number of hole-double pairs at nearest-neighbor distance, one may write for the ground state wave function in this case

$$\psi_o = \sum_{\ell_o+2\ell=N} A_\ell |\ell> \tag{62}$$

with A_ℓ representing the probability amplitude.

The diagonal terms in the Hamiltonian of Equation (14) when operating on the wave function cited above give the following:

$$\frac{\hbar^2\rho^{2/3}}{m}\sum_j b_j^* b_j \psi_o = \frac{\hbar^2\rho^{2/3}}{m} N \psi_o \tag{63}$$

$$\frac{\rho^2 U_o}{2} \sum_j n_j(n_j-1)\psi_o = \rho^2 U_o \sum_\ell \ell A_\ell |\ell> \qquad (64)$$

in which the limitation of no more than double occupancy is imposed. It remains to determine the effect of the off-diagonal term of the Hamiltonian. Thus

$$-\frac{\hbar^2\rho^{2/3}}{2m} \sum_j b_j^*(b_{j+1} + b_{j-1})\,\psi_o = -\frac{\hbar^2\rho^{2/3}}{m}\sqrt{2} \sum_\ell \Big[(N-2\ell)|\ell+1> + \frac{1}{2}\ell|\ell-1>\Big]A_\ell \,. \qquad (65)$$

On the right side of (65), $(N-2\ell)$ replaces ℓ_o by virtue of the constraint of total particle number noted in Equation (62). The factor $\ell/2$ represents the average number of hole-double pairs each of which is destroyed to produce a pair of particles not involved in a hole-double combination; on the average, an equal number of adjacent hole-double pairs are destroyed to create a hole-double pair at second-neighbor distance. These latter are not taken into account in the present analysis.

Introduction of Equations (63) through (65) into the Schrödinger equation gives

$$E\sum_\ell A_\ell|\ell> = \frac{\hbar^2\rho^{2/3}}{m} N\sum_\ell A_\ell|\ell> + \rho^2 U_o \sum_\ell \ell A_\ell|\ell> - \frac{\hbar^2\rho^{2/3}}{m}\sqrt{2}\sum_\ell \Big[(N-2\ell)|\ell+1> + \frac{1}{2}\ell|\ell-1>\Big]A_\ell. \qquad (66)$$

Next multiply both sides of (66) by the orthogonal state vector $\langle n|$ to obtain

$$EA_n = \frac{\hbar^2\rho^{2/3}}{m} N A_n + \rho^2 U_o\, n\, A_n$$

$$- \frac{\hbar^2\rho^{2/3}}{m}\sqrt{2}\left\{\left[N - 2(n-1)\right] A_{n-1} + \frac{1}{2}(n+1)\, A_{n+1}\right\}. \qquad (67)$$

Upon collecting terms and invoking the assumption that $n \gg 1$, one finds from Equation (67)

$$A_n\left[\frac{\hbar^2\rho^{2/3}}{m} + \rho^2 U_o \frac{n}{N} - \frac{E}{N}\right] - \frac{\hbar^2\rho^{2/3}}{m}\sqrt{2}\left[(1-2\frac{n}{N})A_{n-1} + \frac{1}{2}\frac{n}{N} A_{n+1}\right] = 0. \qquad (68)$$

The above difference equation for A_n can most readily be solved by introducing the generating function

$$G(z) = \sum_{n=0}^{\infty} z^n A_n . \qquad (69)$$

Then the terms appearing in Equation (68) can be written as follows:

(a) $$\frac{dG}{dz} = \sum_{n=0}^{\infty} n\, z^{n-1} A_n$$

$$\sum_{n=0}^{\infty} n\, z^n A_n = z\frac{dG}{dz} \qquad (70)$$

(b) $$G = \sum_{n=1}^{\infty} z^{n-1} A_{n-1}$$

$$zG = \sum_{n=1}^{\infty} z^{n} A_{n-1} \tag{71}$$

(c) $$\frac{d}{dz}[zG] = z\frac{dG}{dz} + G = \frac{1}{z}\sum_{n=1}^{\infty} n\, z^{n} A_{n-1}$$

$$\sum_{n=1}^{\infty} n\, z^{n} A_{n-1} = z^{2}\frac{dG}{dz} + zG \tag{72}$$

(d) $$G = \sum_{n=-1}^{\infty} z^{n+1} A_{n+1} \tag{73}$$

$$= A_{o} + z\sum_{n=0}^{\infty} z^{n} A_{n+1}$$

$$\sum_{n=0}^{\infty} z^{n} A_{n+1} = \frac{1}{z}(G - A_{o}) \tag{74}$$

(e) $$\frac{dG}{dz} = \sum_{n=0}^{\infty} (n+1)\, z^{n} A_{n+1} \qquad \text{from (73)}$$

$$= \sum_{n=0}^{\infty} n\, z^{n} A_{n+1} + \sum_{n=0}^{\infty} z^{n} A_{n+1}$$

$$= \sum_{n=0}^{\infty} n\, z^{n} A_{n+1} + \frac{1}{z}(G - A_{o}) \qquad \text{from (74)}$$

$$\sum_{n=0}^{\infty} n\, z^{n} A_{n+1} = \frac{dG}{dz} - \frac{1}{z}(G - A_o) \tag{75}$$

A differential equation for G(z) results when Equations (70) through (75) are substituted into Equation (68):

$$\frac{1}{N}\frac{dG}{dz}\left[\rho^2 U_o z + \frac{\hbar^2\rho^{2/3}}{m} 2\sqrt{2}\, z^2 - \frac{\hbar^2\rho^{2/3}}{m}\frac{\sqrt{2}}{2}\right]$$

$$+ G\left[\frac{\hbar^2\rho^{2/3}}{m} - \frac{E}{N} - \frac{\hbar^2\rho^{2/3}}{m}\sqrt{2}\, z\left(1 - \frac{2}{N}\right) + \frac{\hbar^2\rho^{2/3}}{m}\frac{\sqrt{2}}{2Nz}\right]$$

$$+ \frac{\hbar^2\rho^{2/3}}{m}\frac{\sqrt{2}}{2N} A_o \frac{1}{z} = 0 \,. \tag{76}$$

For large N, certain terms of order $\frac{1}{N}$ can be neglected with respect to terms of much larger magnitude, and one can therefore simplify the expression in (76) to read

$$\frac{1}{N}\frac{dG}{dz}\left[2x\sqrt{2}\, z^2 + z - \frac{x\sqrt{2}}{2}\right] = G\left[\frac{E}{N\rho^2 U_o} - x + x\sqrt{2}\, z\right] \tag{77}$$

where x is defined in Equation (31). In order that ψ_o be normalizable, G(z) can have, in the complex z-plane, no singularity within the unit circle $|z| = 1$ except possibly at the origin. Therefore,

$$2x\sqrt{2}\left[z^2 + \frac{1}{2x\sqrt{2}}\, z - \frac{1}{4}\right] = 0$$

and

$$z = z_1, z_2 = -\frac{1}{4x\sqrt{2}}\left[1 \mp (1 + 8x^2)^{1/2}\right] . \tag{78}$$

Since z_1 is the root for which $|z_1| < 1$,

$$\frac{E}{N\rho^2 U_o} = x - x\sqrt{2}\, z_1$$

whereupon the energy per particle for nearest-neighbor hole-double pairs is

$$\frac{E^n}{N} = \frac{\hbar^2 \rho^{2/3}}{m} \left\{ 1 + \frac{1}{4x} \left[1 - (1 + 8x^2)^{1/2} \right] \right\} . \qquad (79)$$

This result is identical with that obtained by combining Equation (58b) of the previous chapter (giving the energy correction based on propagator modification for nearest-neighbor hole-double combinations) with Equation (27).

To find the probability amplitude A_n of Equation (62), the function $G(z)$ is first determined and subsequently introduced into Equation (69). Let

$$\alpha = - \frac{1}{2x\sqrt{2}} \left[1 - (1 + 8x^2)^{1/2} \right] \qquad (80)$$

whereupon

$$\frac{1}{\alpha} = \frac{1}{2x\sqrt{2}} \left[1 + (1 + 8x^2)^{1/2} \right] .$$

The roots z_1, z_2 of the quadratic equation evaluated earlier can be written

$$z_1 = \frac{\alpha}{2} , \quad z_2 = - \frac{1}{2\alpha} .$$

Equation (77) to be solved for G(z) can now be expressed in the form

$$\frac{1}{N}\frac{dG}{dz} = \frac{1}{2} G \frac{(z-z_1)}{(z-z_1)(z-z_2)}$$

$$= \frac{1}{2} G \frac{1}{z + \frac{1}{2\alpha}} \quad .$$

The solution of the above differential equation is

$$G(z) = C(z + \frac{1}{2\alpha})^{N/2}$$

where C is an integration constant. Choosing $C = (2\alpha)^{N/2}$ such that $A_o = 1$

$$G(z) = (1 + 2\alpha z)^{N/2} \quad . \tag{81}$$

Substitution of (81) into (69) leads to the result

$$A_n = \binom{N/2}{n} (2\alpha)^n \tag{82}$$

whereupon the unnormalized ground state wave function for nearest-neighbor hole-double pairs becomes

$$\psi_o = \sum_{\ell} \binom{N/2}{\ell} (2\alpha)^{\ell} |\ell\rangle \quad . \tag{83}$$

It is of interest to calculate $\langle \ell_o \rangle$ and $\langle \ell \rangle$. Although mathematical complexity prohibits such calculations through the use of (83), reference to Equation (61) of the previous chapter reveals that

$$\langle \ell_o \rangle = \frac{2N}{1 + (1 + 8x^2)^{1/2}} \, . \tag{84}$$

Equation (80) can be solved for x in terms of α and the result introduced into (84). Thus

$$\langle \ell_o \rangle = N(1 - \alpha^2) \, . \tag{85}$$

The constraint on the numbers ℓ_o, ℓ then requires that

$$\langle \ell \rangle = \frac{N}{2} \alpha^2 \, . \tag{86}$$

Since $\alpha \to 0$ as the density becomes extremely large, one observes, as expected, that very few hole-double pairs exist in this limit. On the other hand, as α increases from zero, nearest-neighbor hole-double combinations become increasingly more abundant. The parameter α, therefore, may be regarded as corresponding to the probability amplitude of a hole-double pair at nearest-neighbor distance.

CHAPTER V

GROUND STATE ENERGY FOR A TWO-DIMENSIONAL BOSON SYSTEM

In Chapter III, the entire contribution of linked single pair excitations in the Rayleigh-Schrödinger perturbation theory was ascertained. The procedure followed there was to calculate separately the contribution when a hole does not propagate, when it is considered to propagate one unit cell distance, then two, etc. In each case, the double propagates any number of times, and the total effect of an endless number of double propagations is obtained by analogy with one or more one-dimensional restricted random walk problems. Upon summing to infinite order all the contributions for linked single pairs, one has the result of Equation (39)--namely, that the energy correction can be written in terms of a modified expansion parameter defined in Equation (40). In addition, Equation (39) reveals that, in the final analysis, the entire problem is analogous to a single one-dimensional restricted random walk problem: half the number of paths which begin at the origin and returning thereto after an even number $p(p \geq 2)$ of steps, intermediate returns being prohibited. Thus, from Equations (39) and (40),

$$(\Delta E)^{\ell,s} = \frac{4}{9x}\left(-N\frac{\hbar^2\rho^{2/3}}{m}\right)\sum_{\substack{p=2\\ p\ \text{even}}} C(p-2)\,x^p \qquad (39)$$

$$X = \frac{3}{2} x \tag{40}$$

and x and C(n) are defined respectively by Equations (31) and (34).

In the present chapter, a two-dimensional system of dense Boson particles is considered. One attempts to find the ground state energy of such a system when only linked single pair excitations are counted. A two-dimensional analogue based on the results for the one-dimensional system is readily established. The energy correction given above for a one-dimensional system is derived from Equation (36) of Chapter III which contains a product of two terms, the first indicating the number of possible arrangements of holes and doubles into two groups, the second being derivable from a restricted one-dimensional random walk problem. In the case of a two-dimensional system, the first term should be identical with that arising in one dimension, while the second term should represent a corresponding restricted random walk in two dimensions. This means that the energy correction indicative of linked single pair excitations in two dimensions should have the same form as noted above

$$(\Delta E')^{\ell,s} = \frac{4}{9x} \left(- N \frac{\hbar^2 \rho^{2/3}}{m} \right) S' \tag{87}$$

$$S' = \sum_{\substack{p=2 \\ p \text{ even}}} C'(p-2)\, X^p \tag{88}$$

wherein the prime refers to the fact that a two-dimensional system is under discussion. An evaluation of the right side in (87) is accomplished when C'(p-2) is found. This quantity represents half the number

of rectilinear paths possible on a two-dimensional rectangular lattice, each path returning to the origin after an even number $p(p \geq 2)$ of steps, intermediate returns to the origin being forbidden. Steps here are to be taken parallel to the coordinate axes of the rectangular array.

Solution of the two-dimensional restricted random walk problem mentioned above has not as yet been published in the literature. However, the total number $T(p)$ of possible paths, on a two-dimensional periodic lattice, which start from the origin and return thereto in p steps (with no restrictions on the number of prior passages through the origin) has been found (69) (70) (71):

$$T(p) = \binom{p}{p/2}^2 . \tag{89}$$

The above is simply the square of the value obtained when one considers the identical problem in one dimension. Through the use of (89) one can deduce a reasonable approximation to the energy correction appropriate for linked single pair interactions in a two-dimensional lattice of Bosons. Furthermore, one can derive upper and lower bounds for the energy. The remainder of this chapter is devoted to these calculations.

To begin with, an upper bound to the energy correction in Equation (87) is found as follows. In view of Equation (89) and its relation to the one-dimensional counterpart, one might surmise that the combinatorial number appearing in Equation (88) can be written in a similar manner--namely,

$$2C'(p-2) = \left[2C(p-2)\right]^2 . \tag{90}$$

In other words, since the number of unrestricted paths on a two-dimensional lattice is merely the square of the number for a one-dimensional lattice, the number of restricted paths in two dimensions is similarly the square of the one-dimensional counterpart. However, a little reflection reveals that many more paths are available than those counted in Equation (90). Since the energy correction in Equation (87) is negative, this means that should one employ Equation (90) one would thereby establish an upper bound for the energy correction, and indeed for the energy itself.

With Equation (90) introduced into (88)

$$S_u' = 2\sum_{\substack{p=2 \\ p \text{ even}}} \left[C(p-2)\right]^2 X^p$$

$$S_u' = 8\sum_{\substack{p=2 \\ p \text{ even}}} \frac{1}{p^2}\binom{p-2}{\frac{p}{2}-1}^2 X^p \tag{91}$$

where subscript "u" denotes upper bound. Equation (91) was obtained with the aid of Equation (34). Equation (91) can be rewritten in the form

$$S_u' = 2\sum_{q=1} \frac{1}{q^2}\binom{2q-2}{q-1}^2 X^{2q} . \tag{92}$$

Since

$$\binom{2q-2}{q-1} = \frac{1}{2\pi i}\oint \frac{dy}{y^q}(1+y)^{2q-2}$$

$$\frac{X^{2q}}{q^2} = \frac{2}{q}\int_0^X w^{2q-1}\,dw$$

$$\frac{1}{q} = \int_0^\infty e^{-qu}\, du$$

Equation (92) becomes

$$S_u' = -\frac{1}{\pi^2}\oint \frac{dy}{(1+y)^2}\oint \frac{dz}{(1+z)^2}\int_0^X \frac{dw}{w}\int_0^\infty du \sum_{q=1}\left[\frac{(1+y)^2(1+z)^2}{yz}\, w^2\, e^{-u}\right]^q .$$

$$= -\frac{1}{\pi^2}\oint \frac{dy}{y}\oint \frac{dz}{z}\int_0^X w\, dw \int_0^\infty \frac{du}{e^u - \frac{(1+y)^2}{y}\,\frac{(1+z)^2}{z}\, w^2} . \qquad (93)$$

Upon introducing the substitutions $y = e^{i\phi}$ and $z = e^{i\theta}$, and after integrating in θ and w, one obtains from (93)

$$S_u' = -\frac{1}{2\pi}\int_0^\infty du \int_0^\pi \frac{[1 - 8X^2\, e^{-u}(1 + \cos\phi)]^{1/2} - 1}{1 + \cos\phi}\, d\phi . \qquad (94)$$

With $1 + \cos\phi = 2\cos^2\phi/2 = 2\cos^2\omega$ there results

$$S_u' = -\frac{1}{2\pi}\int_0^\infty du \int_0^{\pi/2} \frac{(1 - 16X^2\, e^{-u}\cos^2\omega)^{1/2} - 1}{\cos^2\omega}\, d\omega . \qquad (95)$$

It is shown in Appendix D that Equation (95) can be expressed in terms of complete elliptic integrals of the first and second kind, K and E,

$$S_u' = \frac{1}{\pi}\left[2E(4X, \tfrac{\pi}{2}) - (1 - 16X^2)K(4X, \tfrac{\pi}{2}) - \tfrac{\pi}{2}\right] . \qquad (96)$$

Finally, this result is introduced into (87), which in turn is combined with E_o as given by (27) to yield an upper bound for the energy per particle:

$$\frac{E_u'}{N} = \frac{\hbar^2\rho^{2/3}}{m}\left\{1 - \frac{2}{9x}\left[\frac{4}{\pi}E(6x, \frac{\pi}{2}) - \frac{2}{\pi}(1-36x^2)K(6x, \frac{\pi}{2}) - 1\right]\right\} \quad (97)$$

in which Equation (40) has been used. A sketch of Equation (97) together with the lower bound as determined below is contained in Chapter VI.

A lower bound on the ground state energy for linked single pairs in a two-dimensional array of particles is based on the following argument. The combinatorial number $C'(p-2)$ in Equation (88) can be taken as that applicable in the two-dimensional unrestricted random walk case and given by Equation (89). Better still, this excessive number of paths can at least be reduced by twice the number of return paths that one would exclude on a one-dimensional lattice. Therefore

$$2C'(p-2) = \binom{p}{p/2}^2 - 2P(p) \quad (98)$$

where $P(p)$ represents those possible paths in one dimension which originate at the origin and terminate again at the origin after p steps, having passed through the origin at least once before termination. This quantity is easily determined. Since the number of possible unrestricted paths in one dimension is the square root of the right side of (89), and since the number of paths terminating at the origin after p steps excluding prior returns is $2C(p-2)$, the difference is

$$P(p) = \binom{p}{p/2}\frac{p-2}{p-1}. \quad (99)$$

Equation (99) is introduced into (98) and this result in turn into Equation (88) to yield

$$S'_{\ell} = \frac{1}{2}\sum_{\substack{p=2 \\ p \text{ even}}} \binom{p}{p/2}^2 X^p - \sum_{\substack{p=2 \\ p \text{ even}}} \binom{p}{p/2} \frac{p-2}{p-1} X^p \tag{100}$$

wherein subscript "ℓ" denotes lower bound. Each of the summations appearing in (100) will be evaluated separately.

The first summation in Equation (100) is

$$S'_{\ell_1} = \sum_{\substack{p=2 \\ p \text{ even}}} \binom{p}{p/2}^2 X^p = \sum_{p=1} \binom{2p}{p}^2 X^{2p} . \tag{101}$$

With

$$\binom{2p}{p} = \frac{1}{2\pi i}\oint \frac{dy}{y^{p+1}} (1+y)^{2p}$$

$$X^{2p} = 2p\int_0^X w^{2p-1}\, dw$$

Equation (101) becomes

$$S'_{\ell_1} = -\frac{1}{2\pi^2}\oint \frac{dy}{y}\oint \frac{dz}{z}\int_0^X \frac{dw}{w}\sum_{p=1} p\left[\frac{(1+y)^2(1+z)^2w^2}{yz}\right]^p . \tag{102}$$

The summation above can be rewritten in closed form. As before, the changes of variable are made: $y = e^{i\phi}$ and $z = e^{i\theta}$. Subsequently, the integrations with regard to ϕ and w are performed. There results

$$S'_{\ell_1} = \frac{1}{\pi}\int_0^{\pi} \frac{d\theta}{\sqrt{1 - 16X^2\cos^2\frac{\theta}{2}}} - 1 . \tag{103}$$

Lastly, the change of variable $\eta = \frac{1}{2}(\pi - \theta)$ reduces the above integral to a complete elliptic integral of the first kind and

$$S'_{\ell_1} = \frac{2}{\pi} K(4X, \frac{\pi}{2}) - 1 \, . \tag{104}$$

In Equation (100), the second summation is

$$S'_{\ell_2} = \sum_{\substack{p=2 \\ p \text{ even}}} \binom{p}{p/2} \frac{p-2}{p-1} X^p$$

$$= 4 \sum_{\substack{p=2 \\ p \text{ even}}} \binom{p-2}{\frac{p}{2}-1} X^p - 4 \sum_{\substack{p=2 \\ p \text{ even}}} \frac{2}{p} \binom{p-2}{\frac{p}{2}-1} X^p \, . \tag{105}$$

Reference to Equation (41) reveals that the second summation above has already been evaluated in considering the one-dimensional random walk problem--that is,

$$\sum_{\substack{p=2 \\ p \text{ even}}} \frac{2}{p} \binom{p-2}{\frac{p}{2}-1} X^p = \frac{1}{2} \left[1 - \sqrt{1 - 4X^2} \right] \tag{106}$$

a result given by Equation (46). Differentiation of the above with respect to X yields for the first summation appearing in (105)

$$\sum_{\substack{p=2 \\ p \text{ even}}} \binom{p-2}{\frac{p}{2}-1} X^p = \frac{X^2}{\sqrt{1 - 4X^2}} \, . \tag{107}$$

Introduction of Equations (106) and (107) into (105) gives

$$S'_{\ell_2} = \frac{4X^2}{\sqrt{1 - 4X^2}} - 2\left[1 - \sqrt{1 - 4X^2}\right] . \qquad (108)$$

Appropriate combination of (104) and (108) as indicated by Equation (100) yields

$$S'_{\ell} = \frac{1}{\pi} K\left(4X, \frac{\pi}{2}\right) - \frac{2(1 - 2X^2)}{\sqrt{1 - 4X^2}} + \frac{3}{2} . \qquad (109)$$

This result when substituted into Equation (87) and the whole combined with E_o produces as a lower bound for the energy per particle

$$\frac{E'_{\ell}}{N} = \frac{\hbar^2 \rho^{2/3}}{m} \left\{1 - \frac{2}{9x}\left[\frac{2}{\pi} K(6x, \frac{\pi}{2}) - 2\frac{2 - 9x^2}{\sqrt{1 - 9x^2}} + 3\right]\right\} . \qquad (110)$$

As mentioned earlier, the upper and lower energy bounds are sketched and discussed in the following chapter.

Having established upper and lower bounds on the ground state energy for linked single pair excitations in a two-dimensional periodic lattice, one now proceeds to determine an approximation for the ground state energy itself. The totality of possible paths in two dimensions which begin at the origin and return to it in p steps, no restrictions on the number of prior passages through the origin, is T(p) and is defined in Equation (89). It was noted before that this result is merely the square of that applicable in the one-dimensional case. The number of possible paths which, in one dimension, originate at the origin and

terminate there in p steps, but which contain the origin as an interior point at least once, is represented by P(p) and is given by Equation (99). It is now assumed that for a two-dimensional lattice the number of return paths can be written as $P^2(p)$. Consequently, the combinatorial number appearing in Equation (88) is found from the relation

$$2C'(p-2) = T(p) - P^2(p) \tag{111}$$

which with the aid of Equations (34), (89), and (99) becomes

$$C'(p-2) = 8\,\frac{(2p-3)}{p^2}\left(\begin{matrix} p-2 \\ \frac{p}{2}-1 \end{matrix}\right)^2 . \tag{112}$$

Equation (112) is introduced into (88) to obtain

$$S'_a = 8\sum_{\substack{p=2 \\ p \text{ even}}} \frac{(2p-3)}{p^2}\left(\begin{matrix} p-2 \\ \frac{p}{2}-1 \end{matrix}\right)^2 X^p$$

$$= 16\sum_{\substack{p=2 \\ p \text{ even}}} \frac{1}{p}\left(\begin{matrix} p-2 \\ \frac{p}{2}-1 \end{matrix}\right)^2 X^p - 24\sum_{\substack{p=2 \\ p \text{ even}}} \frac{1}{p^2}\left(\begin{matrix} p-2 \\ \frac{p}{2}-1 \end{matrix}\right)^2 X^p \tag{113}$$

where subscript "a" refers to the fact that an approximation is being found. The latter summation in (113) is $\frac{1}{8} S'_u$, found with the aid of Equation (91). Differentiation of (91) with respect to X reveals that the first summation in Equation (113) can be written in terms of the derivative of S'_u. Thus

$$S'_a = 2X\frac{dS'_u}{dX} - 3\,S'_u . \tag{114}$$

It is recalled that S_u' has the value cited in Equation (96); differentiation of the elliptic integrals appearing there is accomplished with reference to Jahnke and Emde (72). One therefore obtains from Equation (114)

$$S_a' = \frac{3}{2} - \frac{1}{\pi}\left[4E(4X, \frac{\pi}{2}) - (1 - 16X^2)K(4X, \frac{\pi}{2})\right] . \qquad (115)$$

When this result is introduced into Equation (87), an approximate ground state energy per particle follows:

$$\frac{E_a'}{N} = \frac{\hbar^2\rho^{2/3}}{m}\left\{1 - \frac{2}{9x}\left[3 - \frac{8}{\pi}E(6x, \frac{\pi}{2}) + \frac{2}{\pi}(1 - 36x^2)K(6x, \frac{\pi}{2})\right]\right\} . \qquad (116)$$

The above approximation is contained within the bounds previously calculated and is depicted graphically in the following chapter.

The ground state energy for a two-dimensional system of Bosons has been investigated in this chapter. Linked single pair excitations only were considered. By analogy with the one-dimensional particle array studied in Chapter III, the energy was expressed in terms of a two-dimensional restricted random walk problem. No published solution to this problem has been found by the author. However, an approximate solution for the ground state energy was ascertained and, in fact, an upper and a lower bound on the energy was established. A summary of the results is to be found in Chapter VI, where a synopsis of the calculations based on a one-dimensional model is also presented. It is noted that an analysis similar to that presented in this chapter can be made

for a three-dimensional lattice system. However, due to the lack of known closed-form solutions to three-dimensional random walk problems (except in the asymptotic limit), the results become mathematically unwieldy and, consequently, are not reproduced here.

CHAPTER VI

CONCLUSIONS

Since the binary collision approximation method of Lee and Yang (17) (18), which is based on the introduction of the concept of pseudo-potentials and uses a low-density expansion, cannot be taken seriously for high-density regions, an alternative procedure is required to study the properties of quantum fluids. Although Brueckner and Sawada (8) have applied the formalism developed by Brueckner and Levinson (19)(20) to describe low- and "high"-density properties of a low-temperature Bose-Einstein gas with repulsive particle interactions, the density region which they have considered falls far short of that appropriate in the case of liquids. A cell-model description has frequently been utilized with fairly good success to predict the behavior of classical liquids. Therefore, a quantum mechanical cell model has here been developed for a system of closely-packed Boson particles. Instead of expanding the field operator (expressed in the formalism of second quantization) in a set of plane waves, which diagonalizes in part the Hamiltonian and which is customary at low density, one performs the expansion in a set of Kronecker δ functions. Thereby creation and destruction operators result for particles localized in cells, a description which is almost the inverse of the plane wave formalism. The kinetic energy now has the off-diagonal terms in the representation which diagonalizes the occupation numbers; these terms correspond to

the drifting of particles from cell to cell, resulting in less localization and a consequent decrease in kinetic energy. An effective interaction is realized which depends on density and which, for highly repulsive forces at small volumes, virtually locks particles in their respective cells.

With the Hamiltonian operator taken in the concise formalism of second quantization, a canonical transformation to cell occupation and shift operators has been made. It has been shown that the well-known results for free particles and for low-density Boson systems with interactions can readily be obtained from the transformed Hamiltonian. However, interest here centers on a dense system of Boson particles, and the Hamiltonian is utilized together with the Rayleigh-Schrödinger perturbation theory to calculate the ground state energy of such a system. An exact energy expansion through sixth order of perturbation theory has been presented based on a one-dimensional particle array, wherein both linked and unlinked contributions are taken into account. A consideration of only linked single pair excitations, but to infinite order, selects out of the hierarchy of perturbation terms a particularly simple group, one whose contribution to the ground state energy has been determined precisely. Propagator modification and the ground state wave function applicable in the case of nearest-neighbor hole-double pairs have been determined and utilized to calculate the corresponding contribution to the overall ground state energy. In addition, a Boson system in two dimensions has been studied, for which an approximate energy expansion is derived on the basis of linked single pair excitations; upper and lower bounds on the ground state energy were also determined.

The basic results of the analyses concerning the perturbed ground state energy are summarized in the following equations:

$$\Xi = 1 - x - \frac{1}{4}x^3 - \frac{41}{8}x^5 - - - \tag{117}$$

$$\Xi^{\ell,s} = 1 - \frac{2}{9x}\left(1 - \sqrt{1 - 9x^2}\right) \tag{118}$$

$$\Xi_u^{\prime} = 1 - \frac{2}{9x}\left[\frac{4}{\pi}E(6x, \frac{\pi}{2}) - \frac{2}{\pi}(1 - 36x^2)K(6x, \frac{\pi}{2}) - 1\right] \tag{119}$$

$$\Xi_\ell^{\prime} = 1 - \frac{2}{9x}\left[\frac{2}{\pi}K(6x, \frac{\pi}{2}) - 2\frac{2 - 9x^2}{\sqrt{1 - 9x^2}} + 3\right] \tag{120}$$

$$\Xi_a^{\prime} = 1 - \frac{2}{9x}\left[3 - \frac{8}{\pi}E(6x, \frac{\pi}{2}) + \frac{2}{\pi}(1 - 36x^2)K(6x, \frac{\pi}{2})\right]. \tag{121}$$

In the above, the expansion parameter x is given by

$$x = \frac{\hbar^2\rho^{2/3}}{m\rho^2 U_o} \tag{122}$$

and describes the degree of system confinement; the smaller this parameter the less the wandering of particles throughout the lattice. The energy Ξ in Equations (117) through (121) is the perturbed ground state energy normalized with respect to that of the unperturbed ground state. The latter is given in Equation (27) and is simply the kinetic energy of localization. Equation (117) is the result of an exact calculation through sixth order of perturbation theory and Equation (118) represents

linked single pair excitations to infinite order. Both of these expressions have been determined on the basis of a one-dimensional Boson system of close packing. In two dimensions, upper and lower energy bounds were calculated considering linked single pair excitations; these are given by Equations (119) and (120), respectively. Equation (121) expresses an approximate ground state energy for this latter case.

Figure 10 contains a graph of Equations (117) through (121) wherein the normalized ground state energy is plotted as a function of the expansion or confinement parameter x. A lowering of the energy in a monotonic decreasing fashion is evidenced as more and more particle wanderings occur, a fact which was established at the outset. One notes that the energy calculated on the basis of a two-dimensional particle array is lower than that obtained from the one-dimensional lattice. One would consequently expect even lower energies in the three-dimensional case. A lowering of the energy spectrum with increasing dimensionality of the system is a direct consequence of the concomitant increased freedom afforded the wandering particles. In terms of the Rayleigh-Schrödinger perturbation scheme and related random walk problems, a larger energy correction is obtained the higher the dimensionality due to the larger number of random paths thereby made available. It is of interest in Figure 10 that the energy bounds based on a two-dimensional lattice structure form a relatively narrow energy band, at least over the major portion of the confinement-parameter range.

One notes that the range of the confinement parameter over which the normalized energy for linked single pair excitations in Equation (118) is defined is $0 \leq x \leq \frac{1}{3}$, while that for the normalized energy

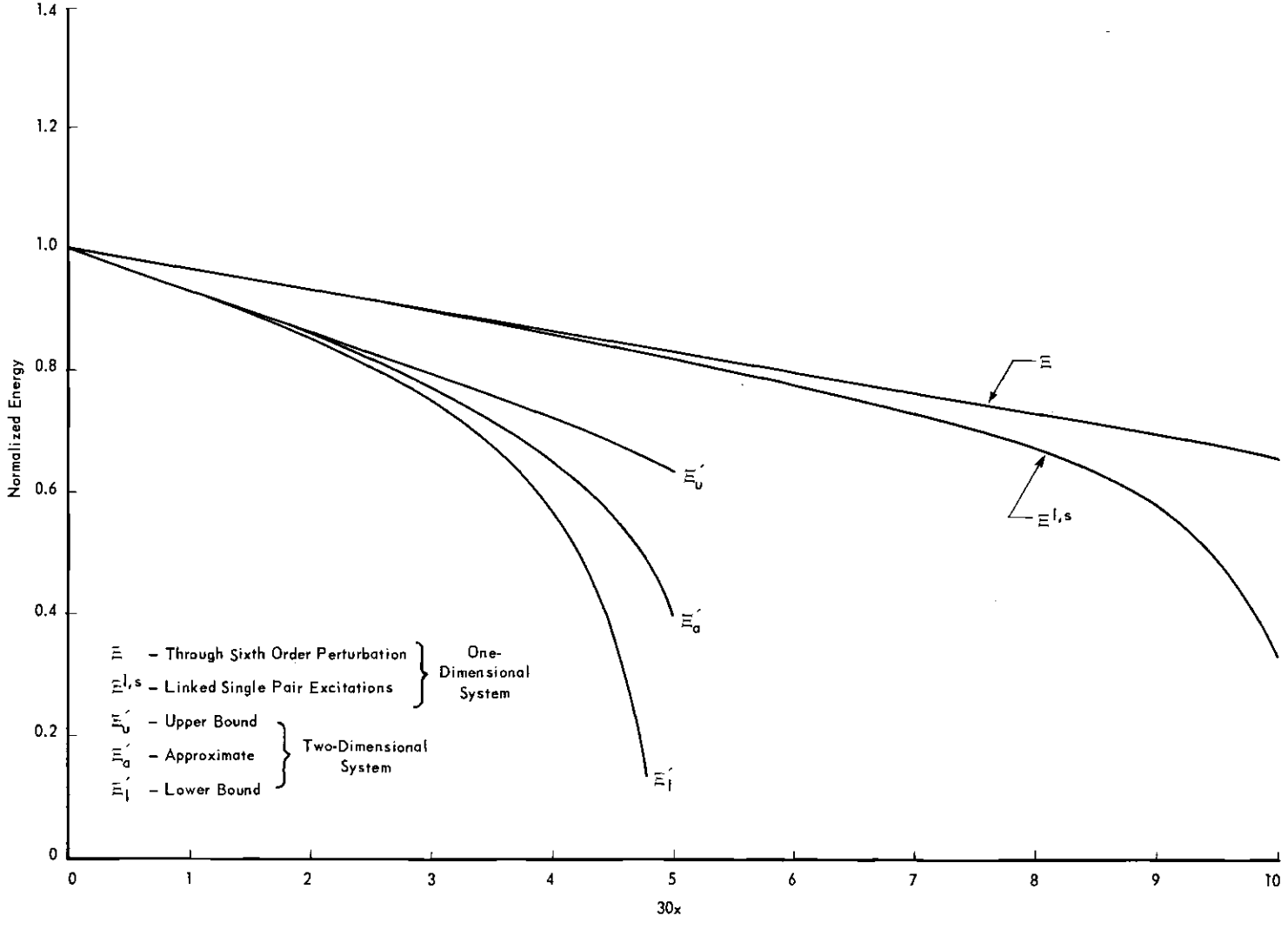


Figure 10. Normalized Ground State Energy for a Dense Boson System Versus Confinement Parameter.

pertaining to a two-dimensional particle array is $0 \leq x \leq \frac{1}{6}$, less by a factor of one half. For a three-dimensional lattice, it is surmised that this range would be smaller still. To ascertain the possible effects of higher oder terms in the perturbation analysis, a calculation was made of the percentage energy change in Equation (117) realized from fourth and sixth order contributions over that obtained from the sum of zero and second order terms. It was found that for x less than a sixth, for example, the added contribution to the normalized ground state energy obtained by including the fourth order perturbation term was less than a sixth of a per cent. The next order in turn contributed only half that contributed by the fourth order correction. Thus, for x no larger than a sixth, the energy is undoubtedly given quite accurately by a calculation merely through second order. For x as large as a third, however, the sixth order contributes an energy correction which amounts to several per cent of that obtained through second order of perturbation. If x is larger still, higher order terms beyond the sixth become increasingly more important.

There follows a discussion concerning the density dependence of Equations (117) through (121); first, though, some additional observations concerning the expansion parameter are in order. From Equations (15a) and (15b) of Chapter II one observes that the effective interaction potential U_o can be written as

$$U_o = \frac{1}{\rho} g(a) \tag{123}$$

where

$$g(o) = \int U(q) d\tau_q \tag{124}$$

and

$$q = |r - r'| \ .$$

Equation (123) is now introduced into the expression for x given in Equation (122); there results

$$x = \frac{\hbar^2 \rho^{2/3}}{m \rho g(o)} \ . \tag{125}$$

As an aid in the subsequent discussion, consider U(q) in (124) to be a potential barrier of height V_o and width a. Then

$$g(o) = \frac{4}{3} \pi V_o a^3$$

and, from Equation (125),

$$x = \frac{3}{4\pi} \frac{1}{S} \frac{1}{\rho^{1/3} a} \tag{126}^{\dagger}$$

where S is dimensionless and represents a measure of the strength of the barrier:

$$S = \frac{m V_o a^2}{\hbar^2} \ .$$

---

†In treating individually one-, two-, and three-dimensional systems, $\rho^{1/3}$ is to be replaced by $\rho^{1-2/n}$ (n=1, 2, 3) so that x is dimensionless in each case. Since a suitable functional dependence of x on ρ is realized only when n = 3, subsequent considerations are restricted to this case.

With x given by Equation (126), one can interpret Figure 10 as a display of normalized ground state energy in terms of interaction strength for fixed density and range of the potential. Density-dependent graphs, on the other hand, are contained in Figure 11, where Equations (117) through (121) are plotted for an interaction strength on the order of unity (specifically, $S = 3/\pi$). Similar statements can be made here as those already applied to Figure 10. In addition, one observes the rather rapid decrease in relative energy as more and more particle migrations occur, or as the density is lowered. For very close packing, linked single pair excitations contribute the dominant amount to the energy obtained through sixth order perturbation theory. However, at lower densities a marked difference is noticed between the respective energy spectra, a fact attesting to the increased importance of multiple pair excitations when at low density. Pressure minima, indicated by points of inflection on certain of the curves depicted in Figure 11, are not to be taken seriously. It is recalled that, for purposes of clarity, a potential barrier has been assumed for the effective interaction. In actuality, the function $g(o)$ in Equation (125) is itself density dependent and could have the effect of modifying the concavity of the curves in the high density region.

To proceed beyond the foundations laid by the present study, one must devise a mathematical approach to the three-dimensional Boson case. It has already been noted that to relate the energy correction in this case to restricted random walks on periodic, three-dimensional lattices is extremely difficult at present since solutions to such problems are conspicuously absent from the literature. A very promising venture and one which has briefly engaged this author's attention concerns the

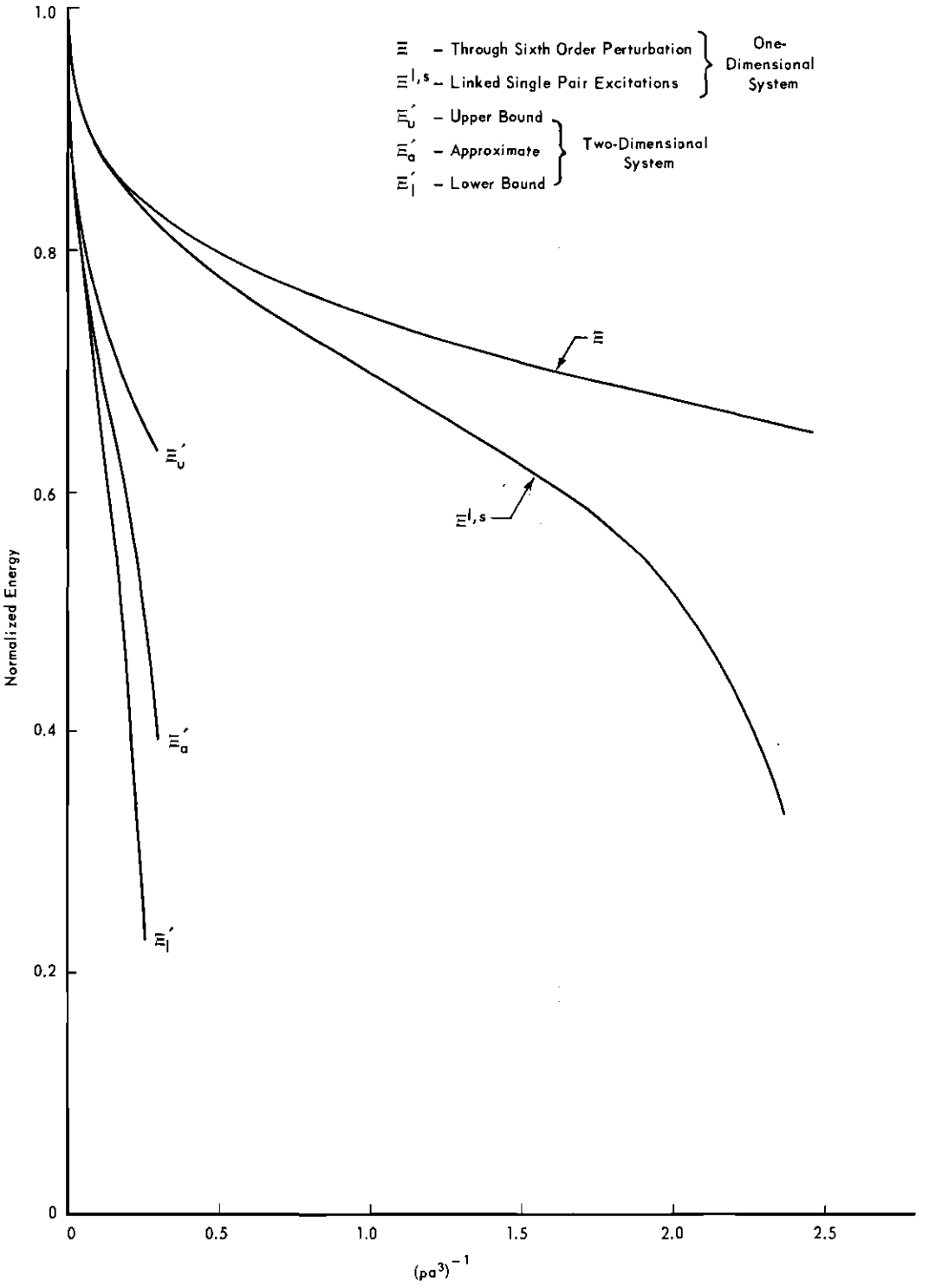


Figure 11. Normalized Ground State Energy for a Dense Boson System as a Function of Reciprocal Density.

determination of a unitary transformation which will diagonalize the cell-model Hamiltonian of Chapter II. Another fruitful approach may be by way of the variational principle introduced into the many-body problem by Bogoliubov (73). It is further noted that an improved description of a close-packed system can be realized by including a finer spatial scale than that considered herein. This would involve a choice for the function $f(r - r_j)$ in Equation (4) which would include some fluctuations within a cell volume. Attention should also be given to the form of the ground state wave function with which to describe the overall system, especially if one is to be concerned with excited states. It may be pointed out, finally, that sufficient progress has been made on the rearranged perturbation series for linked multiple pairs, such as those of Figure 5, to indicate that these also can be summed to infinite order in much the same fashion as was done for linked single pairs.

APPENDIX A

CELL-MODEL HAMILTONIAN AND THE PHONON SPECTRUM

An outline of the procedures leading from the Hamiltonian applicable for the cell model postulated herein to the well-known phonon spectrum (60) (61) (62) is contained in Chapter II. Details of the mathematical manipulations involved are presented below.

With the introduction into the Hamiltonian, Equation (14), of the approximation

$$b_{r_j} = 1 + \xi_{r_j}$$

and considering the ξ's to be sufficiently small compared to unity such that the products of three or more may be neglected, one obtains

$$H = \frac{N\rho^2 U_o}{2} + \frac{\hbar^2 \rho^{2/3}}{2m} \sum_{r_j} (2\xi^*_{r_j}\xi_{r_j} - \xi^*_{r_j}\xi_{r_j+r_o} - \xi^*_{r_j}\xi_{r_j-r_o})$$

$$+ \frac{\rho^2 U_o}{2} \sum_{r_j} (\xi^*_{r_j}\xi^*_{r_j} + \xi_{r_j}\xi_{r_j} + 2\xi^*_{r_j}\xi_{r_j})$$

$$+ \frac{\hbar^2 \rho^{2/3}}{2m} \sum_{r_j} (2\xi_{r_j} - \xi_{r_j+r_o} - \xi_{r_j-r_o})$$

$$+ \rho^2 U_o \sum_{r_j} (\xi^*_{r_j} + \xi_{r_j} + \xi^*_{r_j}\xi_{r_j}) \; . \qquad \text{(A1)}$$

The last term above is zero, as evidenced by application of the inverse transformation to this term:

$$\sum_{r_j} (\xi^*_{r_j} + \xi_{r_j} + \xi^*_{r_j} \xi_{r_j}) = \sum_{r_j} (b^*_{r_j} b_{r_j} - 1)$$

$$= \sum_{r_j} b^*_{r_j} b_{r_j} - N$$

$$= 0$$

where the last step involves the use of Equation (8). Equation (A1) now reduces to Equation (22) of Chapter II with the exception of the second last term. This latter term is also zero, a fact which will presently become evident.

The transformation of (A1) to plane wave operators is now made through the relationship

$$\xi_{r_j} = \frac{1}{\sqrt{N}} \sum_k a_k e^{ik \cdot r_j} .$$

By the same procedures as followed in Equations (16) through (18a) in Chapter II one arrives at the Hamiltonian in the new form

$$H = \frac{N\rho^2 U_o}{2} + \frac{\hbar^2 \rho^{2/3}}{m} \sum_k \left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) a_k^* a_k$$

$$+ \frac{\rho^2 U_o}{2} \sum_k (a_k^* a_{-k}^* + a_k a_{-k})$$

$$+ \frac{\hbar^2}{2m} \sqrt{N} \sum_k k^2 a_k \delta_{k,o} \quad . \tag{A2}$$

The last term in (A2) is obviously zero, leaving a result which is Equation (23) in Chapter II.

Equation (7) expresses a commutation relation pertaining to the operator b_{r_j}. It is easily verified that the operators ξ_{r_j} in Equation (A1) and a_k in (A2) obey identical commutation rules. A further canonical transformation is now presented--namely,

$$a_k = u_k \eta_k + v_k \eta_{-k}^*$$

in which the η_k and η_k^* are new Boson operators and $u_k = u_{-k}$, $v_k = v_{-k}$; the latter are c-number functions of k such that (74)

$$u_k^2 - v_k^2 = 1 \quad . \tag{A3}$$

The Hamiltonian (A2) transforms as follows in terms of the newly introduced operators:

$$H = \frac{N\rho^2 U_o}{2} + \sum_k \left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) \times$$

$$[u_k^2 \, \eta_k^* \, \eta_k + u_k \, v_k (\eta_{-k} \, \eta_k + \eta_k^* \, \eta_{-k}^*) + v_k^2 \, \eta_{-k} \, \eta_{-k}^*]$$

$$+ \frac{\rho^2 U_o}{2} \sum_k [u_k^2 (\eta_k^* \, \eta_{-k}^* + \eta_k \, \eta_{-k})$$

$$+ u_k \, v_k (\eta_{-k} \, \eta_{-k}^* + \eta_k^* \, \eta_k + \eta_{-k}^* \, \eta_{-k} + \eta_k \, \eta_k^*)$$

$$+ v_k^2 (\eta_{-k} \, \eta_k + \eta_{-k}^* \, \eta_k^*)] \, .$$

Application of the commutation rule to the terms $\eta\eta^*$ permits one to write

$$H = H_o + H_1 + H_2$$

where

$$H_o = \frac{N\rho^2 U_o}{2} + \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) v_k^2 + \rho^2 U_o \, u_k \, v_k \right] \qquad (A4)$$

$$H_1 = \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) \left(u_k^2 + v_k^2 \right) + 2\rho^2 U_o \, u_k \, v_k \right] \eta_k^* \, \eta_k \qquad (A5)$$

$$H_2 = \sum_k \left[\left(\frac{\hbar^2 k^2}{2m} + \rho^2 U_o \right) u_k v_k + \frac{\rho^2 U_o}{2} \left(u_k^2 + v_k^2 \right) \right] \times$$

$$\left(\eta_k^* \eta_{-k}^* + \eta_k \eta_{-k} \right) . \qquad \text{(A6)}$$

Since the last transformation is to diagonalize the Hamiltonian and thus give the energy H_o of the ground state and that of the excited states H_1, Equation (A6) is set equal to zero:

$$2 \left(1 + \frac{\hbar^2 k^2}{2m\rho^2 U_o} \right) u_k v_k + u_k^2 + v_k^2 = 0 . \qquad \text{(A7)}$$

Thus Equations (A3) and (A7) may be solved simultaneously to determine u_k and v_k. There results

$$u_k = \frac{1}{\sqrt{1 - L_k^2}}$$

$$v_k = \frac{L_k}{\sqrt{1 - L_k^2}}$$

where

$$L_k = - \left(1 + \frac{\hbar^2 k^2}{2m\rho^2 U_o} \right) + \left[\left(1 + \frac{\hbar^2 k^2}{2m\rho^2 U_o} \right)^2 - 1 \right]^{1/2} .$$

When the above expressions are introduced into Equation (A5) the phonon spectrum cited in Chapter II is obtained:

$$H_1 = \sum_k \mathcal{E}_k \, \eta_k^* \, \eta_k$$

$$\mathcal{E}_k = \left(\frac{\hbar^2 k^2}{2m} \right)^{1/2} \left(\frac{\hbar^2 k^2}{2m} + 2\rho^2 U_o \right)^{1/2} .$$

APPENDIX B

RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY

A fairly detailed exposition of bound state perturbation theory in terms of the compact symbolic language characteristic of abstract operator formalism found in quantum field theories has been published by DeWitt (63). It is the purpose here to outline the fundamental procedures leading to an expression, in this general formalism, of the Rayleigh-Schrödinger perturbation formula, which specifies the changes in the discrete energy levels of a system when a small disturbance is applied, and which is the basis of the perturbation calculation in Chapter III of the text.

The Hamiltonian operator for the system of interest is denoted by H, where the latter is assumed from the outset to be separable into a part H_o of sufficiently simple structure so that its Schrödinger equation can be solved, and another part H_1 small enough so that it can be regarded as a perturbation on H_o. To "switch on" a quantum state abruptly, Green's functions $G_o(t, t')$ and $G(t, t')$ for the respective systems H_o and H are introduced. These satisfy the time-dependent Schrödinger equation as follows:

$$(i\hbar \frac{\partial}{\partial t} - H_o)G_o(t, t') = i\hbar\delta(t - t') \qquad (B1)$$

$$(i\hbar \frac{\partial}{\partial t} - H)G(t, t') = i\hbar\delta(t - t') \ . \qquad (B2)$$

If neither H_o nor H has any explicit dependence on t, then Equations (B1) and (B2) yield

$$G_o(t,\ t') = \Theta(t,\ t')\ e^{-\frac{i}{\hbar} H_o(t-t')} \tag{B3}$$

$$G(t,\ t') = \Theta(t,\ t')\ e^{-\frac{i}{\hbar} H(t-t')} \tag{B4}$$

where

$$\Theta(t,\ t') = \frac{1}{2}\left(1 + \frac{t - t'}{|t - t'|}\right) . \tag{B5}$$

The functions G_o and G depend only on the difference between the times t and t'. Setting t' = 0 and taking the Fourier transform of (B3) and (B4) one has

$$G_o(E) = \int_{-\infty}^{\infty} G_o(t,\ 0)\ e^{\frac{i}{\hbar} Et}\ dt = \frac{1}{E - H_o} \tag{B6}$$

$$G(E) = \int_{-\infty}^{\infty} G(t,\ 0)\ e^{\frac{i}{\hbar} Et}\ dt = \frac{1}{E - H} . \tag{B7}$$

Since $H = H_o + H_1$, Equation (B7) can be written in the form

$$G(E) = [(E - H_o) + (- H_1)]^{-1} = (A + B)^{-1} . \tag{B8}$$

From the identity

$$(A + B)^{-1}\ (A + B) = 1$$

or

$$(A + B)^{-1}\ A + (A + B)^{-1}\ B = 1$$

$$(A + B)^{-1} AA^{-1} = [1 - (A + B)^{-1} B]A^{-1}$$

$$(A + B)^{-1} = [1 - (A + B)^{-1} B]A^{-1}$$

Equation (B8) can be expressed as

$$G(E) = [1 + G(E)H_1]G_o(E) \quad . \tag{B9}$$

Formal solution of the above yields $G(E)$ in terms of $G_o(E)$ as follows:

$$G(E) = G_o(E)[1 - H_1 G_o(E)]^{-1} \quad . \tag{B10}$$

The discreteness of the bound-state energy levels enables one to stipulate that the singularities of the Green's function operators $G_o(E)$ and $G(E)$ in the complex E-plane will be separate simple poles. Each singularity $H_o^{(i)}$ of $G_o(E)$ may, for example, be enclosed by a separate contour $C^{(i)}$ in such a way that the regions surrounded by the contours do not overlap. Then, the following projection operators are defined:

$$P_o^{(i)} = \frac{1}{2\pi i} \oint_{C^{(i)}} G_o(E)\, dE \tag{B11}$$

$$P^{(i)} = \frac{1}{2\pi i} \oint_{C^{(i)}} G(E)\, dE \quad . \tag{B12}$$

In addition, a level shift operator $\Delta^{(i)}$ is given by

$$\Delta^{(i)} = \frac{1}{2\pi i} \oint_{C^{(i)}} (E - H_o^{(i)}) G(E)\, dE. \qquad (B13)$$

The aforementioned operators play the basic roles in bound state perturbation theory.

Equation (B13) is used to find the energy level shifts due to the perturbation. In the notation employed before in Equation (B8)

$$(A + B)(A + B)^{-1} = 1$$

$$(A + B)G(E) = 1$$

$$AG(E) = 1 - BG(E)$$

$$(E - H_o)G(E) = 1 + H_1 G(E)$$

$$= 1 + (H - H_o)G(E) \,. \qquad (B14)$$

In virtue of the identity in (B14) it is evident that (B13) reduces to

$$\Delta^{(i)} = (H - H_o^{(i)}) \frac{1}{2\pi i} \oint_{C^{(i)}} G(E)\, dE$$

which through (B12) is simply

$$\Delta^{(i)} = (H - H_o^{(i)}) P^{(i)} = \Delta E^{(i)}\, P^{(i)} \qquad (B15)$$

where the $\Delta E^{(i)}$ are the level shifts. The operators $\Delta^{(i)}$ are thus seen to be simple multiples of the projection operators $P^{(i)}$. Now, the energy level shifts may be computed from the relation

$$\Delta E^{(i)} = \mathrm{Tr}\, \Delta^{(i)} \quad . \tag{B16}$$

Introduction of Equation (B10) into (B13) and substitution of the resulting expression for $\Delta^{(i)}$ into (B16) gives

$$\Delta E^{(i)} = \mathrm{Tr}\, \frac{1}{2\pi i} \oint_{C^{(i)}} (E - H_o^{(i)}) G_o(E) [1 - H_1 G_o(E)]^{-1}\, dE \quad . \tag{B17}$$

It is noted that the integral in (B17) can be evaluated by separating out the singularity of $G_o(E)$ at $H_o^{(i)}$. One may write for $G_o(E)$

$$\begin{aligned} G_o(E) &= \frac{P_o^{(i)}}{E - H_o} + \frac{1 - P_o^{(i)}}{E - H_o} \\ &= \frac{P_o^{(i)}}{E - H_o^{(i)}} + \frac{1 - P_o^{(i)}}{H_o^{(i)} - H_o} \left(1 + \frac{E - H_o^{(i)}}{H_o^{(i)} - H_o} \right)^{-1} \\ &= -\frac{g_o}{z} + \frac{\beta}{y} \left(1 + \frac{z}{y} \right)^{-1} \quad . \end{aligned}$$

By expanding the bracketed inverse and introducing the whole into (B17) one obtains

$$\Delta E^{(i)} = \mathrm{Tr}\, \frac{1}{2\pi i} \oint_{C^{(i)}} z\, dz \left[-\frac{g_o}{z} + \frac{\beta}{y} \sum_{\ell=0} \left(-\frac{z}{y} \right)^{\ell} \right] \times \left[1 - H_1 \left(-\frac{g_o}{z} + \frac{\beta}{y} \sum_{\ell=0} \left(-\frac{z}{y} \right)^{\ell} \right) \right]^{-1} \tag{B18}$$

where

$$g_o = - P_o^{(i)} \qquad \beta = 1 - P_o^{(i)}$$

$$y = H_o^{(i)} - H_o \qquad z = E - H_o^{(i)} \, .$$

A further expansion this time of the bracketed inverse in (B18), and a selection of the terms in z^{-1} for integration (all others vanish when integrated) leads to

$$\Delta E^{(i)} = \mathrm{Tr} \sum_{n=1}^{\infty} \sum_{\substack{k_i \geq 0 \\ k_1+k_2+\cdots+k_{n+1}=n-1}} g_{k_1} H_1 g_{k_2} H_1 \cdots H_1 g_{k_{n+1}} \tag{B19}$$

where

$$g_k = \frac{\beta}{y^k} = \frac{1 - P_o^{(i)}}{(H_o^{(i)} - H_o)^k} \, . \tag{B20}$$

Since the trace in (B19) is invariant to cyclic permutation, one can write

$$\Delta E^{(i)} = \sum_{n=1}^{\infty} \sum_{\substack{k_i \geq 0 \\ k_1+k_2+\cdots+k_n=n-1}} (k_n - 1) \, \mathrm{Tr} \, H_1 g_{k_1} H_1 g_{k_2} \cdots H_1 g_{k_n} \, . \tag{B21}$$

This equation may be further simplified through the observation that the factors occurring in the summand can be cyclically rearranged in n different orders, each giving the same result. One of these orders is chosen

as standard and is then the only order allowed in the summation. The numerical factor preceding the trace must thus be replaced by

$$\sum_{i=1}^{n} (k_i - 1) = \sum_{i=1}^{n} k_i - n = (n-1) - n = -1.$$

Choosing the standard order to be that for which $k_n = 0$, one finds that there are N_k other orders which meet this specification, N_k being the number of remaining indices k_i, $i < n$, which are equal to zero. Each of these orders may be regarded as equally standard if a factor $(N_k+1)^{-1}$ is inserted. Therefore Equation (B21) takes the final form

$$\Delta E^{(i)} = \sum_{n=1} \sum_{\substack{k_i \geq 0 \\ k_1+k_2+\cdots+k_n=n-1}} (N_k+1)^{-1} \langle i | H_1 \, g_{k_1} \, H_1 \, g_{k_2} \cdots g_{k_{n-1}} \, H_1 | i \rangle$$

which is known as the Rayleigh-Schrödinger perturbation formula and leads to Equation (28) of the text. The trace symbol has been eliminated by the assumption that H_1 has been diagonalized within the subspace $P^{(i)}$.

APPENDIX C

EVALUATION OF THE GENERAL GROUP IN THE SUM (35)

It was pointed out in Chapter III that each group of terms in the sum (35) has the value $C(m+1)$, where $C(n)$ is defined by Equation (34). The proof of this statement consists in writing and evaluating the general or q-th group. Since the verification is identical for q even or odd, the even case only is considered.

Accordingly, the q-th group of (35) has a sum Q which can be expressed as follows:

$$Q = \sum_{\substack{v=1 \\ v \text{ odd}}}^{q+1} C(-v,\ m-q,\ -v-1)\ [C(v-1,\ q,\ -1) + C(v+1,\ q,\ -1)]\ . \qquad (C1)$$

This expression is rewritten in terms of binomial coefficients with the help of Equation (33):

$$Q = \sum_{\substack{v=1 \\ v \text{ odd}}}^{q+1} \left[\binom{m-q}{\frac{1}{2}(m-q-v)} - \binom{m-q}{\frac{1}{2}(m-q-v-2)} \right]$$

$$\left[\binom{q}{\frac{1}{2}(q-v+1)} - \binom{q}{\frac{1}{2}(q-v-2)} \right]$$

$$Q = \sum_{\substack{v=1 \\ v \text{ odd}}}^{q+1} \binom{m-q}{\frac{1}{2}(m-q-v)} \binom{q}{\frac{1}{2}(q-v+1)}$$

$$+ \sum_{\substack{v=1 \\ v \text{ odd}}}^{q-3} \binom{m-q}{\frac{1}{2}(m-q-v-2)} \binom{q}{\frac{1}{2}(q-v-3)}$$

$$- \Bigg[\sum_{\substack{v=1 \\ v \text{ odd}}}^{q+1} \binom{m-q}{\frac{1}{2}(m-q-v-2)} \binom{q}{\frac{1}{2}(q-v+1)}$$

$$+ \sum_{\substack{v=1 \\ v \text{ odd}}}^{q-3} \binom{m-q}{\frac{1}{2}(m-q-v)} \binom{q}{\frac{1}{2}(q-v-3)} \Bigg] . \qquad (C2)$$

Substitution of $k = \frac{1}{2}(q-v+1)$ in the first and third terms of (C2) and $k = \frac{1}{2}(q-v-1)$ in the second and fourth gives

$$Q = \sum_{k=0}^{q/2} \binom{a}{t+k} \binom{q}{k} + \sum_{k=1}^{\frac{q}{2}-1} \binom{a}{t+k} \binom{q}{k-1}$$

$$- \Bigg[\sum_{k=0}^{q/2} \binom{a}{t-1+k} \binom{q}{k} + \sum_{k=1}^{\frac{q}{2}-1} \binom{a}{t+1+k} \binom{q}{k-1} \Bigg] ; \qquad (C3)$$

where

$$a = m-q$$

$$t = \frac{1}{2}(a-q-1) \ .$$

To evaluate the indicated sums above, reference is made to Feller (75) who notes that

$$\sum_{k=0}^{b} \binom{a}{t+k}\binom{b}{k} = \binom{a+b}{a-t} \ . \qquad (C4)$$

Equation (C4) can be written

$$\sum_{k=0}^{b/2} \binom{a}{t+k}\binom{b}{k} + \sum_{k=\frac{b}{2}+1}^{b} \binom{a}{t+k}\binom{b}{k} = \binom{a+b}{a-t} \qquad (C5)$$

where the second sum is expressible by

$$R = \sum_{k=\frac{b}{2}+1}^{b} \binom{a}{t+k}\binom{b}{k} = \sum_{k=\frac{b}{2}+1}^{b} \binom{a}{a-t-k}\binom{b}{b-k} \ . \qquad (C6)$$

Substitution of $s = b-k+1$ in Equation (C6) produces

$$R = \sum_{s=1}^{b/2} \binom{a}{a-t-b-1+s}\binom{b}{s-1} = \sum_{s=1}^{b/2} \binom{a}{t+s}\binom{b}{s-1} \qquad (C7)$$

this latter provided $t = \frac{1}{2}(a-b-1)$. Under this condition, then, Equation (C5) has the form

$$\sum_{k=0}^{b/2}\binom{a}{t+k}\binom{b}{k}+\sum_{k=1}^{b/2}\binom{a}{t+k}\binom{b}{k-1} = \binom{a+b}{a-t} . \qquad (C8)$$

However, for $t = \frac{1}{2}(a-b-3)$, Equation (C7) becomes

$$R = \sum_{s=1}^{b/2}\binom{a}{t+2+s}\binom{b}{s-1}$$

and (C5) can be written

$$\sum_{k=0}^{b/2}\binom{a}{t+k}\binom{b}{k}+\sum_{k=1}^{b/2}\binom{a}{t+2+k}\binom{b}{k-1} = \binom{a+b}{a-t} . \qquad (C9)$$

With $t = w - 1$, the above equation becomes

$$\sum_{k=0}^{b/2}\binom{a}{w-1+k}\binom{b}{k}+\sum_{k=1}^{b/2}\binom{a}{w+1+k}\binom{b}{k-1} = \binom{a+b}{a-w+1} \qquad (C10)$$

a result valid when $w = \frac{1}{2}(a-b-1)$.

Returning to Equation (C3), one finds formulas (C8) and (C10) to be directly applicable. Hence

$$Q = \binom{a+q}{a-t} - \binom{a}{t+\frac{q}{2}}\binom{q}{\frac{q}{2}-1}$$

$$- \left[\binom{a+q}{a-t+1} - \binom{a}{t+1+\frac{q}{2}}\binom{q}{\frac{q}{2}-1} \right]$$

$$= \binom{m}{\frac{1}{2}(m+1)} - \binom{m-q}{\frac{1}{2}(m-q-1)}\binom{q}{\frac{q}{2}-1}$$

$$- \binom{m}{\frac{1}{2}(m+3)} + \binom{m-q}{\frac{1}{2}(m-q+1)}\binom{q}{\frac{q}{2}-1}$$

$$= \binom{m}{\frac{1}{2}(m+1)} - \binom{m}{\frac{1}{2}(m+3)}$$

$$= \frac{2}{m+3} \cdot \frac{(m+1)!}{\left[\frac{1}{2}(m+1)\right]!^2} .$$

Reference to Equation (34) in Chapter III expressing the definition of C(n) reveals that Q can be abbreviated as

$$Q = C(m+1)$$

the result which was to be verified.

APPENDIX D

DERIVATION OF EQUATION (96)

Equation (95) of the text reads

$$S'_u = -\frac{1}{2\pi}\int_0^\infty I(u, X)\, du \tag{D1}$$

where

$$I(u, X) = \int_0^{\pi/2} \frac{(1-k^2\cos^2\omega)^{1/2} - 1}{\cos^2\omega}\, d\omega \tag{D2}$$

and

$$k = 4X\, e^{-\frac{u}{2}} \,. \tag{D3}$$

To evaluate the integral in Equation (D2), let $\omega = \frac{\pi}{2} - \beta$. Then

$$I(u, X) = \int_0^{\pi/2} \frac{(1-k^2\sin^2\beta)^{1/2}}{\sin^2\beta} - \int_0^{\pi/2} \csc^2\beta\, d\beta \,.$$

Integrating the first integral by parts, one has

$$I(u, X) = -k^2 \int_0^{\pi/2} \frac{\cos^2\beta}{\sqrt{1-k^2\sin^2\beta}}\, d\beta \,. \tag{D4}$$

Reference to Jahnke and Emde (76) reveals that

$$I(u, X) = -k^2 B(k) \tag{D5}$$

where B(k) is a function involving elliptic integrals of the first and second kinds and can be written as

$$B(k) = (1 - \frac{1}{k^2})K(k) + \frac{1}{k^2} E(k) \quad . \tag{D6}$$

Substitution of (D5) into Equation (D1) gives

$$S'_u = \frac{1}{2\pi} \int_0^{16X^2} B(s)\, ds \quad .$$

Again reference is made to Jahnke and Emde (77) to obtain

$$S'_u = \frac{1}{\pi} [E(4X, \frac{\pi}{2}) + 16X^2\, B(4X, \frac{\pi}{2}) - \frac{\pi}{2}] \tag{D7}$$

where E is a complete elliptic integral of the second kind. When the function B appearing in Equation (D7) is replaced by its equivalent expressed by (D6), Equation (96) of the text ensues:

$$S'_u = \frac{1}{\pi} [2E(4X, \frac{\pi}{2}) - (1 - 16X^2)K(4X, \frac{\pi}{2}) - \frac{\pi}{2}] \quad .$$

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VITA

Gilbert Carl Knollman was born in Cleveland, Ohio, on March 14, 1928. He was valedictorian of John Marshall High School in Cleveland in 1945. After spending an academic year at Case Institute of Technology, he served in the U. S. Counter Intelligence Corps, spending a year in Germany as Special Agent. He received the Bachelor of Science degree in 1949 and the Master of Science degree in 1950, both from the Georgia Institute of Technology. In 1950, he joined the staff of the Engineering Experiment Station as Assistant Research Physicist and was promoted to Research Physicist in 1953. In addition to his full-time engagement in classified military research, he has been associated with the School of Physics and has instructed in the School of Mathematics for eight years. He is the author or co-author of twenty technical publications in various fields of physics and applied mathematics, and is a member of Sigma Xi and the American Physical Society.